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# Spectroscopic Constants for Selected Homonuclear Diatomic Molecules

## Volume II. K Through Z

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16 February 1976

Interim Report

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P.O. Box 92960, Worldway Postal Center  
Los Angeles, Calif. 90009

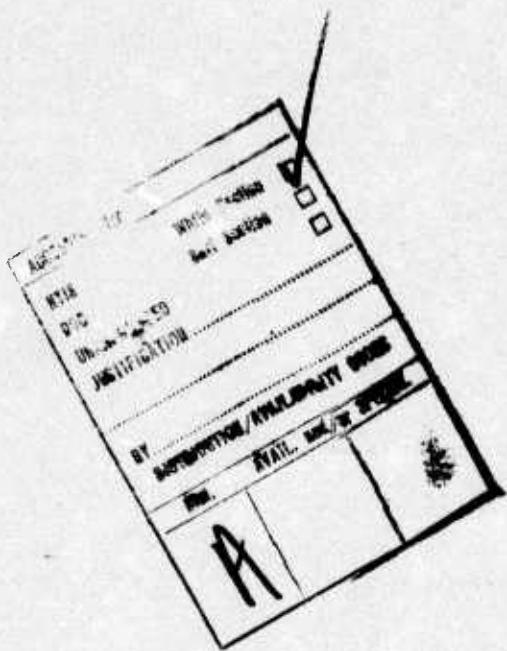
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This report was submitted by The Aerospace Corporation, El Segundo, CA 90245, under Contract F04701-75-C-0076 with the Space and Missile Systems Organization, Deputy for Advanced Space Programs, P.O. Box 92960, Worldway Postal Center, Los Angeles, CA 90009. It was reviewed and approved for The Aerospace Corporation by W. R. Warren, Jr., Director, Aerophysics Laboratory. Lt. Ronald C. Lawson, USAF, was the project officer. This research was supported by the Defense Advanced Research Projects Agency of the Department of Defense.

This report has been reviewed by the Information Office (OI) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nations.

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

## REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS  
BEFORE COMPLETING FORM

3. RECIPIENT'S CATALOG NUMBER

## 1. REPORT NUMBER

SAMSO-TR-76-31 Vol 52

## 2. GOVT ACCESSION NO.

6. TITLE (and subtitle)  
SPECTROSCOPIC CONSTANTS FOR SELECTED  
HOMONUCLEAR DIATOMIC MOLECULES,  
Volume II. K Through Z

## 5. TYPE OF REPORT &amp; PERIOD COVERED

9. Interim Rept.,

## 6. PERFORMING ORG. ACTIVITY NUMBER

14. TR-0076(6751)-1 Vol 52

## 7. CONTRACT OR GRANT NUMBER(s)

15. F04701-75-C-0076

DARPA Order 2-2843

## 7. AUTHOR(s)

10. Steven N. Suchard James E. Melzer

## 9. PERFORMING ORGANIZATION NAME AND ADDRESS

The Aerospace Corporation  
El Segundo, Calif. 90245

## 10. PROGRAM ELEMENT, PROJECT, TASK AREA &amp; WORK UNIT NUMBERS

12. 229p,

## 11. CONTROLLING OFFICE NAME AND ADDRESS

Defense Advanced Research Projects Agency  
1400 Wilson Blvd.  
Arlington, Va. 22209

## 11. REPORT DATE

16 Feb 1976

## 12. NUMBER OF PAGES

272

13. SECURITY CLASS. (of this report)  
Unclassified14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)  
Space and Missile Systems Organization  
Air Force Systems Command  
Los Angeles, Calif. 90009

## 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

## 16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

## 17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

## 18. SUPPLEMENTARY NOTES

## 19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Branching Ratio  
Electron Transition  
Electronic Quenching Rate  
Franck-Condon Factor

## 20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Spectroscopic information relevant to homonuclear diatomic molecules has been collected and is presented. This information includes not only the molecular band systems, but also Frank-Condon factors, oscillator strengths, potential energy curves, and reactive branching ratios, where available.

The information is arranged alphabetically by molecule in two volumes. This. the second volume, covers K through Z.

DD FORM 1473  
(FACSIMILE)

409 367

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1B

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**SECURITY CLASSIFICATION OF THIS PAGE(When Data Entered)**

**19. KEY WORDS (Continued)**

Molecular Band System  
Potential Energy Diagram  
Radiative Lifetime  
Reaction Rate  
Spectroscopic Constant  
Spectroscopy

**20. ABSTRACT (Continued)**

**UNCLASSIFIED**

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## PREFACE

During the preparation of this compilation, many people contributed; the compilers wish to thank all of them. In particular they appreciate the efforts of V. Gilbertson, the manuscript typist; and K. C. Bregand, J. A. Kiley, and W. H. McPherson, for their editorial assistance. They would like to thank Dr. J. R. Schwartz for his cooperation and encouragement. In addition, they extend their gratitude to Dr. L. Wilson of the Air Force Weapons Laboratory, who gave the initial impetus to this project.

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## I. INTRODUCTION

A complete discussion of the purpose, organization, and notation used in this compilation and comments on the availability of spectroscopic information are presented in Volume I of this report. The only intent here is to outline the text of Volume I, to which the reader is referred.

Generally, the information on the alphabetically arranged molecules is broken into five separate sections: viz., methods of production and experimental technique, band systems, spectroscopic constants, perturbations and general information, and bibliography. These are described briefly.

### METHODS OF PRODUCTION AND EXPERIMENTAL TECHNIQUE

Sources for the production of the molecule and techniques for study are presented.

### BAND SYSTEMS

A general description is given of the molecular transition of each system or group. The system is analyzed in detail.

### SPECTROSCOPIC CONSTANTS

The molecular constants that totally define the electronic states of the molecule are given. The bulk of the dissociation energy information is taken from Gaydon (Ref. 7 in Vol I); other sources are so noted.

### PERTURBATIONS AND GENERAL INFORMATION

All other information deemed useful to the complete understanding of the molecule is included here.

### BIBLIOGRAPHY

The referencing system (after Suchard, Ref. 4 in Vol I) is made up of two numbers: first, the year of publication; second, the running count of references cited for each molecule.

Also presented in Volume I is a section "Notation and Notational Conversion Formulas." Formulas are given for such molecular properties as total energy of a given state of the molecule T, electronic energy  $T_e$ , vibrational energy G, and rotational energy F. Nomenclature for other molecular constants reported is also given.

MOLECULE	VIBRA-	ROTA-	VIBRA-	DISSO-	FRANCK-	BRANCH-	QUENCH-	LASER ACTION
	TIONAL CONSTANTS	TIONAL CONSTANTS	TIONAL LEVEL DISTRIBU-	CIATION ENERGY	CONDOON FACTORS	ING RATIOS		OBSERVED
$\text{Ac}_2$								
$\text{Ag}_2$	X				X			
$\text{Al}_2$	X	X			X			
$\text{Am}_2$								
$\text{Ar}_2$	P	P			X			X
$\text{As}_2$	X	X			X	P	P	
$\text{At}_2$								
$\text{Au}_2$	X	X			X	P		
$\text{B}_2$	X	X			X			
$\text{Ba}_2$								
$\text{Be}_2$					P			
$\text{Bi}_2$	X	P			X			
$\text{Bk}_2$								
$\text{Br}_2$	X	X	P	X	P	X		P
$\text{C}_2$	X	X	P	X	X			
$\text{Ca}_2$	P	P		X				
$\text{Cd}_2$					X			
$\text{Ce}_2$					X			
$\text{Cl}_2$	X	P		X		P		P
$\text{Cm}_2$								
$\text{Co}_2$					X			
$\text{Cr}_2$					X			
$\text{Cs}_2$	X			X	P			

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-1

MOLECULE	VIBRA-	ROTA-	VIBRA-	DISSO-	LIFE-	FRANCK-	BRANCH-	QUENCH-	LASER ACTION OBSERVED	
	TIONAL CONSTANTS	TIONAL CONSTANTS	LEVEL DISTRIBU-	CIACTION ENERGY	TIMES	CONDON FACTORS	RATIOS		VIBRA-	ELEC-
$\text{Cu}_2$	X	P		X		P				
$\text{Dy}_2$					X					
$\text{Er}_2$					X					
$\text{Es}_2$										
$\text{Eu}_2$					X					
$\text{F}_2$	P	P			X					
$\text{Fe}_2$					X					
$\text{Fm}_2$										
$\text{Fr}_2$					X					
$\text{Ga}_2$										
$\text{Gd}_2$					X					
$\text{Ge}_2$					X					
$\text{H}_2$	X	X	P	X	X	X		X		X
$\text{He}_2$	X	X		X						X
$\text{Hf}_2$										
$\text{Hg}_2$					X					
$\text{Ho}_2$										
$\text{I}_2$	X	X	P	X	P	X		X		X
$\text{In}_2$	X			P						
$\text{Ir}_2$										
$\text{K}_2$	X	P		X	P					
$\text{Kr}_2$	X	P		X						X
$\text{La}_2$	P			X						
$\text{Li}_2$	X	X		X	P					

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-2

MOLECULE	VIBRA-TIONAL CONSTANTS	ROTA-TIONAL CONSTANTS	VIBRA-TIONAL LEVEL DISTRIBUTIONS	OISSO-CIATION ENERGY	LIFE-TIMES	FRANCK-CONDON FACTORS	BRANCH-ING RATIOS	QUENCH-ING	VIBRA-TIONAL	ELEC-TRONIC	LASER ACTION OBSERVED
Lu <sub>2</sub>											
Md <sub>2</sub>											
Mg <sub>2</sub>	X	X			X		X				
Mn <sub>2</sub>					X						
Mo <sub>2</sub>											
N <sub>2</sub>	X	X	P	X	X	X			X		X
Na <sub>2</sub>	X	X		X	P	P					
Nb <sub>2</sub>					X						
Nd <sub>2</sub>					X						
Ne <sub>2</sub>	P	P		X	P						
Ni <sub>2</sub>					X						
No <sub>2</sub>											
Np <sub>2</sub>											
O <sub>2</sub>	X	X	P	X	X	X			X		
Os <sub>2</sub>											
P <sub>2</sub>	X	P		X					P		
Pa <sub>2</sub>											
Pb <sub>2</sub>	X			X							
Pd <sub>2</sub>					X						
Pm <sub>2</sub>											
Po <sub>2</sub>		X			X						
Pr <sub>2</sub>						X					
Pt <sub>2</sub>											
Pu <sub>2</sub>											

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-3

MOLECULE	VIBRA-	ROTA-	VIBRA-	DISSO-	LIFE-	FRANCK-	BRANCH-	QUENCH-	LASER ACTION
	TIONAL CONSTANTS	TIONAL CONSTANTS	TIONAL LEVEL DISTRIBU-	CIATION ENERGY	TIMES	CONON FACTORS	ING RATIOS	ING	OBERVED
R <sub>a</sub> <sub>2</sub>									
R <sub>b</sub> <sub>2</sub>	X			X	P			P	
R <sub>e</sub> <sub>2</sub>									
R <sub>h</sub> <sub>2</sub>									
R <sub>n</sub> <sub>2</sub>									
R <sub>u</sub> <sub>2</sub>									
S <sub>2</sub>	X	X		X	P			P	
S <sub>b</sub> <sub>2</sub>	X	P		X				P	
S <sub>c</sub> <sub>2</sub>				X					
S <sub>e</sub> <sub>2</sub>	X	X		X				P	
S <sub>i</sub> <sub>2</sub>	X	X		X				P	
S <sub>m</sub> <sub>2</sub>				X					
S <sub>n</sub> <sub>2</sub>				X					
S <sub>r</sub> <sub>2</sub>									
T <sub>a</sub> <sub>2</sub>									
T <sub>b</sub> <sub>2</sub>				X					
T <sub>c</sub> <sub>2</sub>									
T <sub>e</sub> <sub>2</sub>	X	X		X		X			
T <sub>h</sub> <sub>2</sub>				X					
T <sub>i</sub> <sub>2</sub>				X					
T <sub>l</sub> <sub>2</sub>				X					
T <sub>m</sub> <sub>2</sub>				X					
U <sub>2</sub>				X					
V <sub>2</sub>				X					

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-4

MOLECULE	VIBRA-TIONAL CONSTANTS	ROTA-TIONAL CONSTANTS	VIBRA-TIONAL LEVEL DISTRIBUTIONS	DISSO-CIATION ENERGY	LIFE-TIMES	FRANCK-CONDON FACTORS	BRANCH-ING RATIOS	QUENCH-ING	LASER ACTION OBSERVED	
									VIBRA-TIONAL	ELEC-TRONIC
W <sub>2</sub>										
Xe <sub>2</sub>	P				X	P		P		X
Y <sub>2</sub>					X					
Yb <sub>2</sub>					X					
Zn <sub>2</sub>					P					
Zr <sub>2</sub>										

X=SUBSTANTIAL INFORMATION; P=SKETCHY INFORMATION; NO NOTATION=NO INFORMATION

Chart II-5

K<sub>2</sub>Methods of Production and Experimental Technique**Absorption.****Emission from a heat pipe, laser fluorescence.****BAND SYSTEMS**

System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
I	$A^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	Heat Pipe	8850-7700	R			(71.47, 30.10)
II	$B^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption, laser fluores- cence	6950-6250	R	6583. 2(0, 2) 6544. 0(0, 1) 6473. 6(1, 0)		(68.39, 32.15, 31.12)
III	$C^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption	4510-4220	R	4343. 5(1, 0)		(61.32, 48.29)
IV	$D(^1\Pi_u) \leftarrow X^1\Sigma_g^+$	Absorption	4160-3940	R	4082. 7(1, 2)		(48.29)
V	$E(^1\Pi_u) \leftarrow X^1\Sigma_g^+$	Absorption	3925-3700	R	3797. 6(2, 3) 3793. 7(1, 2)		(50.31)
VI	$F \leftarrow X^1\Sigma_g^+$	Absorption	3700-3600	R			(37.20, 37.19)
VII	$G \leftarrow X^1\Sigma_g^+$	Absorption	3600-3480	R			(37.19)

Molecule K<sub>2</sub>

K<sub>2</sub>

I.  $A^1\Sigma_u^+ \approx X^1\Sigma_g^+$  System

Most characteristic bands,  $\lambda$  (30.10):

(v', v'')	(0, 3)	(0, 2)	(1, 2)	(0, 1)	(0, 0)	(1, 0)	(2, 0)
$\lambda$	8773.15	8702.00	8651.79	8634.43	8566.30	8515.70	8468.23

II.  $B^1\Pi_u \approx X^1\Sigma_g^+$  System

Most intense band heads,  $\lambda$  (Intensity) (32.15, 31.12):

v', v''	(0, 2)	(0, 1)	(1, 1)	(1, 0)	(2, 0)
$\lambda$	6583.19	6544.00	6512.19	6473.58	6443.00
(Intensity)	9	8	5	10	8

III.  $C^1\Pi_u \approx X^1\Sigma_g^+$  System

Most intense band heads,  $\lambda$  (Intensity) (61.32, 48.29):

v', v''	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
$\lambda$	4355.1	4343.5	4332.3	4320.9	4310.0
(Intensity)	8	10	7	7	7

IV.  $D\left(^1\Pi_u\right) \leftarrow X^1\Sigma_g^+$  System

Possibly two independent systems,  $\lambda$  (Intensity) (27.20, 37.19):

v', v''	0	1	2	3	4	5
0			4092.3(8)	4107.3(7)	4122.7(6)	
1		4067.0(8)	4082.7(10)	4097.4(7)	4112.8(8)	
2				4087.5(6)	4103.0(6)	
3	4033.5(6)			4078.2(6)		4108.6(6)
4	4024.9(6)					

V.  $E(^1\Pi_u) \leftarrow X^1\Sigma_g^+ System$

Most intense band heads,  $\lambda$  (Intensity) (50.31):

$v', v''$	0	1	2	3
0				
1			3793.7(10)	3806.2(7)
2		3771.5(8)	3784.4(7)	3797.6(10)
3		3762.8(7)	3776.0(7)	3789.2(7)
4				
5	3733.8(7)	3746.6(7)		
6		3738.1(7)		

VI.  $F \leftarrow X^1\Sigma_g^+ System$

Most intense band heads, analysis uncertain,  $\lambda$  (37.20, 37.19):

$v', v''$	0	1	2	3
0		3639.5	3651.7	
1		3631.6	3643.4	
2	3611.2	3623.5	3635.3	3647.3
3	3603.2			

VII.  $G \leftarrow X^1\Sigma_g^+ System$

Most intense band heads,  $\lambda$  (Intensity) (37.19):

$(v', v'')$	$(0, 2)$	$(1, 2)$	$(2, 2)$	$(3, 2)$	$(4, 2)$	$(3, 1)$	$(4, 1)$
$\lambda$ (Intensity)	3583.7 4	3575.6 4	3567.6 4	3559.9 3	3553.4 4	3548.6 3	3541.1 3

SPECTROSCOPIC CONSTANTS

Molecule  $K_2$

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e \times 10^2$	$\alpha_e \times 10^{-4}$	$D_e \times 10^{-8}$	$r_e$	Remarks	Bibliography
G	28091	64.9	0.05						(37.19)
F	27571	62.2	0.24						(37.19)
E ( $^1\Pi_u$ )	26493.0	60.6	0.15						(50.31)
D ( $^1\Pi_u$ )	24627.7	61.6	0.90						(a) (4.8.29)
C $^1\Pi_u$	22969.7	61.48	0.14	4.404	1.10	4.43			(61.32, 50.31)
B $^1\Pi_u$	15376.4	92.021	0.2829	5.6743	1.65	8.63	4.23	(b) (68.39, 32.15, 31.13)	
A $^1\Sigma_u^+$	11682.6	69.09	0.153						(30.10)
X $^1\Sigma_g^+$	0	92.64		5.622	2.19	8.28	3.92	(c) (61.32, 48.29)	

(a)  $y_e \omega_{ee} = 0.001$ ,  $z_e \omega_{ee} = -0.0003$ ; (b)  $y_e \omega_{ee} = -0.002055$ ,  $\gamma_e = -7.2 \times 10^{-6}$ ,  $\delta_e = 1.5 \times 10^{-7}$ ,  $\beta = -7.4 \times 10^{-10}$ ;

(c)  $\beta = -8.3 \times 10^{-11}$

Dissociation energy =  $0.51 \pm 0.05$  eV, 11.8 kcal/mole,  $4114 \text{ cm}^{-1}$ .

$K_{-4}$

Perturbations and General Information

Radiative lifetime of B<sup>1</sup> $\Pi_u$  state (70.44, 70.41):

$$\tau(B^1\Pi_u) = 9.65 \pm 0.3 \text{ nsec.}$$

Absolute absorption cross sections (68.37, 66.35).

Potential energy curves, RKR potentials (69.40):

	State	v	U(cm <sup>-1</sup> )	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)
T <sub>e</sub> = 0.0	X <sup>1</sup> $\Sigma_g^+$	0	46.2	3.7906	4.0643
		1	138.2	3.6996	4.1752
		2	229.4	3.6394	4.2554
		3	319.9	3.5918	4.3230
		4	409.7	3.5516	4.3835
		5	498.8	3.5164	4.4391
		6	587.2	3.4848	4.4912
		7	674.9	3.4560	4.5407
		8	761.9	3.4294	4.5880
		9	848.1	3.4047	4.6337
		10	933.7	3.3815	4.6780
		11	1018.5	3.3597	4.7212
		12	1102.7	3.3389	4.7633
		13	1186.1	3.3192	4.8047
		14	1268.9	3.3003	4.8453
		15	1350.9	3.2822	4.8852
T <sub>e</sub> = 15376.4 cm <sup>-1</sup>	B <sup>1</sup> $\Pi_u$	0	37.4	4.0886	4.3929
		1	111.6	3.9885	4.5179
		2	185.1	3.9225	4.6089
		3	257.9	3.8706	4.6861
		4	330.0	3.8269	4.7553
		5	401.3	3.7886	4.8192
		6	472.0	3.7544	4.8794
		7	542.0	3.7233	4.9367
		8	611.2	3.6945	4.9917
		9	679.8	3.6678	5.0451
		10	747.6	3.6427	5.0970
		11	814.7	3.6190	5.1478
		12	881.0	3.5965	5.1978
		13	946.5	3.5749	5.2471
		14	1011.2	3.5542	5.2959
		15	1075.1	3.5341	5.3445

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- (32. 14) B ← X System,  
F. W. Loomis,  
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Kr<sub>2</sub>Methods of Production and Experimental TechniqueAbsorption.

Emission: positive columns, condensed discharge, microwave discharge, electron beam discharge,  $\alpha$ -particle irradiation.

## BAND SYSTEMS

System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
I	$1,3\Sigma_u^- \rightarrow 1\Sigma_g^+$	$\sigma$ irradiation	1250-1850	V	Max. $\sim 1480\text{\AA}$ , 1280 $\text{\AA}$	Continuum	(73.9, 65.4, 55.3, 55.2)
	$B(1_u^-) \rightarrow X 1\Sigma_g^+(0^+)$	Absorption	1252-1257		1254.8(3, 4)		(73.10)
	$C(0_u^+) \rightarrow X 1\Sigma_g^+(0^+)$	Absorption	1239-1245		1241.3(3, 4) 1242.3(4, 4)		(73.10)
	$D(0_u^+) \rightarrow X 1\Sigma_g^+(0^+)$	Absorption	1167-1169		1168.1(2, 0) 1167.6(4, 1)		(73.10)
	$E \rightarrow X 1\Sigma_g^+$	Absorption	1161-1170				(73.10)
		Emission	2000-8000			Continuum	(67.7, 42.1)
			1064-1080			4 fragmented systems	(73.10)

Systems II - V correlate to separated atom limits in which one atom is excited to various levels of configuration  $4p^55s$ .

System VII systems are energetically close to various atom levels of configuration  $4p^55p$ .

**Kr<sub>2</sub>**

II. B(1<sub>u</sub>) - X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>(0<sub>g</sub><sup>+</sup>) System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0				1252. 3(2)	
1			1252. 8(2)	1253. 1(6)	
2			1253. 7(6)	1253. 9(8)	
3	1254. 0(1)		1254. 6(8)	1254. 8(10)	
4	1255. 0(0)		1255. 6(1)	1255. 8(3)	

III. C(0<sub>u</sub><sup>+</sup>) - X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>(0<sub>g</sub><sup>+</sup>) System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0				1239. 2(9)	1239. 5(9)
1		1239. 2(9)	1239. 5(7)	1239. 8(8)	1240. 0(10)
2	1239. 6(6)	1239. 9(7)	1240. 2(8)	1240. 4(8)	1240. 7(9)
3	1240. 2(4)	1240. 6(4)	1240. 9(5)	1241. 1(6)	1241. 3(10)
4	1241. 0(1)	1241. 4(3)	1241. 6(5)	1241. 9(8)	1242. 1(10)

IV. D(0<sub>u</sub><sup>+</sup>) - X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>(0<sub>g</sub><sup>+</sup>) System

Band heads, λ (Intensity) (73.10):

v', v''	0	1	2	3	4
0	1169. 2(5)	1169. 5(4)	1169. 7(3)	1170. 0(2)	1170. 1(1)
1	1168. 6(8)	1168. 9(5)	1169. 2(5)	1169. 4(2)	1169. 6(2)
2	1168. 1(8)	1168. 4(2)	1168. 7(3)	1168. 9(5)	1169. 1(3)
3	1167. 7(6)	1168. 0(7)	1168. 2(2)	1168. 4(2)	1168. 7(3)
4	1167. 3(7)	1167. 6(8)	1167. 8(5)		1168. 2(2)

V. E - X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> System

Band heads in absorption, λ (Intensity) (73.10):

λ (Intensity)	1161. 4 10	1162. 3 9	1163. 1 8	1163. 7 7	1164. 1 6	1164. 4 6
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## SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$D(0_u^+)$	85531.5	(a) 39.66 (b)							(73.10)
$C(0_u^+)$	80763.9	(a) 35.75 (b)							(73.10)
$B(1_u)$	79932.8	22.3 (b)							(73.10)
$X^1\Sigma_g^+$ ( $0_g^+$ )	0	23.99	1.3	0.024	1.0			$y_e w_e = 0.021$	(73.11, 73.10)

(a)  $T_o$ ; (b)  $\Delta G_{1/2}$ Dissociation energy = 0.02 eV, 0.3° kcal/mole, 138.4 cm<sup>-1</sup> (73.10).

Kr<sub>2</sub>

Perturbations and General Information

Laser action has been observed on the  ${}^1, {}^3\Sigma_u^+ \rightarrow X {}^1\Sigma_g^+$  transition at  $1457 \pm 8\text{\AA}$  (73.13).

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La<sub>2</sub>Methods of Production and Experimental Technique

Thermal emission from a King furnace ( $T > 2000^{\circ}\text{C}$ ).

Band Systems

Bands in the region 6100-6040 Å have been attributed to La<sub>2</sub>. The bands are degraded principally to the violet, but the series convergence is degraded red (69.2).

Characteristic bands:

$\lambda | 6075.3 | 6074.9 | 6074.7 | 6074.6 | 6069.4 | 6068.8 | 6049.6 | 6049.1$

A vibrational analysis yields  $\omega'_o = 82.6 \text{ cm}^{-1}$  and  $\omega''_o = 76.9 \text{ cm}^{-1}$ , but these values are in doubt.

Spectroscopic Constants

Dissociation energy =  $2.50 \pm 0.22 \text{ eV}$ ,  $57.6 \text{ kcal/mole}$ ,  $20200 \text{ cm}^{-1}$  (64.1).

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Li<sub>2</sub>Methods of Production and Experimental Technique

Absorption, magnetic rotation.

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
	I	A <sup>1</sup> $\Sigma_u^+$ - X <sup>1</sup> $\Sigma_g^+$	Absorption	7700-6550	R	6883. 9(2, 0)		(72.64, 29.16, 28. I)
	II	B <sup>1</sup> $\Pi_u$ - X <sup>1</sup> $\Sigma_g^+$	Absorption	5590-4500	R	4800. 6(3, 1) 4778. 8(2, 0)		(33.13, 31.9)
	III	C <sup>1</sup> $\Pi_u$ - X <sup>1</sup> $\Sigma_g^+$	Absorption	3500-3100	R	3358. 6(0, 2) 3315. 6(0, I)		(60.36, 38.3I)
	IV	D <sup>1</sup> $\Gamma_u$ - X <sup>1</sup> $\Sigma_g^+$	Absorption	3100-2500	R			(60. 36)

Several bands of the isotopic species <sup>7</sup>Li<sup>6</sup>Li have been observed for Systems II and III.

Molecule Li<sub>2</sub>

$\text{Li}_2$

I.  $A^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$  System

Most intense band heads,  $\lambda$  (Intensity) (36.16, 28.1):

$(v', v'')$	$(0, 2)$	$(0, 1)$	$(1, 1)$	$(1, 0)$	$(2, 0)$	$(3, 0)$
$\lambda$	7690.3	7309.2	7177.4	7003.7	6883.9	6768.7
(Intensity)	8	8	8	8	10	8

II.  $B^1\Pi_u \leftarrow X^1\Sigma_g^+$  System

Most intense band heads of  ${}^7\text{Li}_2$ ,  $\lambda$  (Intensity) (31.9):

$(v', v'')$	$(2, 1)$	$(1, 0)$	$(3, 1)$	$(2, 0)$	$(4, 1)$	$(3, 0)$
$\lambda$	4859.7	4838.2	4800.6	4778.8	4744.9	4722.0
(Intensity)	1.5	4	10	10	4	1.5

Most intense band heads of  ${}^7\text{Li} {}^6\text{Li}$ ,  $\lambda$  (Intensity) (31.9):

$(v', v'')$	$(0, 0)$	$(1, 0)$	$(4, 1)$
$\lambda$	4901.8	4836.5	4739.7
(Intensity)	5	4	2

III.  $C^1\Pi_u \leftarrow X^1\Sigma_g^+$  System

Most intense band heads,  $\lambda$  (Intensity) (60.36, 48.31):

$(v', v'')$	$(0, 4)$	$(1, 4)$	$(0, 3)$	$(2, 4)$	$(0, 2)$	$(0, 1)$	$(0, 0)$	$(1, 0)$
$\lambda$	3431.2	3404.4	3392.1	3378.5	3358.6	3315.6	3277.6	3253.1
(Intensity)	4	4	6	4	10	9	6	10

IV.  $D^1\Pi_u \leftarrow X^1\Sigma_g^+$  System

Several systems are superimposed in the region 3100-2500 Å. Simple Q branches here have been attributed to a  $D^1\Pi_u \leftarrow X^1\Sigma_g^+$  system. The D state appears perturbed (60.36).

## SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$D^1\Pi_u$	$\leq 34140$	$\sim 205$		0.465			3.18		(60.36)
$C^1\Pi_u$	30549	237.9	3.33	0.5068	9.39	9.9	3.08	$y_e w_e = 0.060$	(60.36)
$B^1\Pi_u$	20439.40	270.94	3.13	0.5577	8.88	9.45	2.93	$y_e w_e = -0.0637$	(33.13, 3.9)
$A^1\Sigma^+_u$	14069.9	255.50	1.59	0.4975	5.22		3.11	$y_e w_e = 0.0039^{(a)}$	(36.16, 28.1)
$X^1\Sigma^+_g$	0	351.43	2.55	0.672	6.8	9.87	2.67	(b)	(69.51, 36.16, 28.1)

(a) Spectroscopic constants for  ${}^6\text{Li}_2$  (72.64); (b) spectroscopic constants for  ${}^6\text{Li}_2$ ,  ${}^7\text{Li} {}^6\text{Li}$  (69.31)

Dissociation energy =  $1.026 \pm 0.006$  eV, 23.66 kcal/mole,  $8275 \text{ cm}^{-1}$  (69.51).

**Li<sub>2</sub>**

**Perturbations and General Information**

Gyromagnetic ratio ( $g_j$ ) = 0.10797 nuclear magnetons (64.39).

Transition probabilities (70.53):

Transition	v	f
A <sup>1</sup> $\Sigma_u^+$ - X <sup>1</sup> $\Sigma_u^+$	14068	0.8688

C <sup>1</sup> $\Pi_u$ - X <sup>1</sup> $\Sigma_u^+$	30558	0.0158
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Average polarizability (990°K) =  $34 \times 10^{-24}$  cm<sup>3</sup> (74.68).

Potential energy curves - RKR potentials (69.50):

	State	v	U(cm <sup>-1</sup> )	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)
T <sub>e</sub> = 0.0	X <sup>1</sup> $\Sigma_g^+$	0	175.1	2.5163	2.8480
		1	521.3	2.4131	2.9911
		2	862.3	2.3470	3.0980
		3	1198.0	2.2961	3.1906
		4	1528.4	2.2542	3.2752
		5	1853.5	2.2183	3.3548
		6	2173.2	2.1868	3.4309
		7	2487.5	2.1588	3.5046
		8	2796.4	2.1336	3.5766
		9	3099.7	2.1107	3.6475
		10	3397.6	2.0897	3.7175
		11	3689.9	2.0704	3.7872
		12	3976.6	2.0526	3.8566
		13	4257.7	2.0361	3.9260
		14	4533.2	2.0203	3.9956
		15	4802.9	2.0066	4.0656
		16	5067.0	1.9935	4.1361
T <sub>e</sub> = 14069.9 cm <sup>-1</sup>	A <sup>1</sup> $\Sigma_u^+$	0	127.3	2.9237	3.3125
		1	379.7	2.8043	3.4812
		2	628.8	2.7281	3.6066
		3	874.9	2.6693	3.7142
		4	1117.9	2.6205	3.8116
		5	1357.7	2.5782	3.9021

State	v	U(cm <sup>-1</sup> )	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)
$T_e = 20439.40 \text{ cm}^{-1}$	B <sup>1</sup> $\Pi_u$	0	134.2	2.7598
		1	398.2	2.6448
		2	656.1	2.5714
		3	907.6	2.5148
		4	1152.2	2.4675
		5	1389.7	2.4263
		6	1619.6	2.3893
		7	1841.5	2.3552
		8	2055.0	2.3232
		9	2259.8	2.2927
		10	2455.5	2.2631
		11	2641.7	2.2339
		12	2814.6	2.2016
		13	2976.8	2.1704
		14	3127.9	2.1384

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Mg<sub>2</sub>

Mg<sub>2</sub>

Methods of Production and Experimental Technique

Absorption (T ~ 800° C).

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
	I	$A^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Absorption	3853-3140	V	3790. 9(0, 2) 3764. 7(0, 3)		(70.7)
	II	$(^1\Pi_u) \leftarrow X^1\Sigma_g^+$	Absorption	2852-2660	-			(70.7)

Molecule Mg<sub>2</sub>

I. A<sup>1Σ<sup>+</sup></sup> ← X<sup>1Σ<sup>+</sup> g System</sup>

Band heads, λ (70.7):

v', v''	3	4	5	6	7
2	3790. 9	3796. 5	3801. 6	3806. 3	3810. 7
3	3764. 6	3770. 2	3775. 3	3779. 9	3784. 2
4	3739. 2	3744. 5	3749. 5	3754. 2	3758. 3
5	3714. 2	3719. 5	3724. 5	3729. 0	

## SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$A^1\Sigma_u^+$	26068.76	190.6151.14562	0.147999		1.31642	0.334286	3.082		(70.7)
$X^1\Sigma_g^+$	0	51.12	1.6448	0.0929	3.7758	1.2166	3.890		(70.7)

Dissociation energy = 0.05 eV, 1.15 kcal/mole,  $404.1 \text{ cm}^{-1}$  (73.19).

**Mg<sub>2</sub>**

**Perturbations and General Information**

Potential energy curves - RKR potentials (72.8):

T <sub>e</sub>	State	v	E(v) cm <sup>-1</sup>	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)
T <sub>e</sub> = 0.0	X <sup>1Σ<sup>+</sup><sub>g</sub></sup>	0	25. 156	3. 6872	4. 1626
		1	73. 037	3. 5698	4. 4165
		2	117. 757	3. 5010	4. 6260
		3	159. 384	3. 4509	4. 8226
		4	197. 971	3. 4112	5. 0166
		5	233. 558	3. 3786	5. 2140
		6	266. 168	3. 3513	5. 4195
		7	295. 811	3. 3285	5. 6380
		8	322. 482	4. 4097	5. 8750
		9	346. 162	3. 2948	6. 1378
		10	366. 806	3. 2835	6. 4364
		11	384. 393	3. 2762	6. 7852
		12	398. 831	3. 2717	7. 2110
T <sub>e</sub> = 26068.76 cm <sup>-1</sup>	A <sup>1Σ<sup>+</sup><sub>u</sub></sup>	0	95. 021	2. 9676	3. 2111
		1	283. 350	2. 8915	3. 3154
		2	469. 404	2. 8426	3. 3927
		3	653. 193	2. 8048	3. 4591
		4	834. 728	2. 7736	3. 5193
		5	1014. 020	2. 7467	3. 5754
		6	1191. 078	2. 7231	3. 6286
		7	1365. 915	2. 7018	3. 6796
		8	1538. 541	2. 6826	3. 7290
		9	1708. 965	2. 6649	3. 7771
		10	1877. 199	2. 6486	3. 8242
		11	2043. 254	2. 6335	3. 8704
		12	2207. 139	2. 6193	3. 9150
		13	2368. 867	2. 6060	3. 9609
		14	2528. 446	2. 5935	4. 0055
		15	2685. 889	2. 5818	4. 0497

## Franck-Condon factors - RKR potentials (72.8):

 $A^1\Sigma_u^+ - X^1\Sigma_g^+$ 

v', v''	0	1	2	3	4	5	6	7	8
0	0.0000	0.0000	0.0001	0.0003	0.0006	0.0010	0.0014	0.0019	0.0022
1	0.0001	0.0004	0.0012	0.0027	0.0047	0.0070	0.0092	0.0110	0.0121
2	0.0004	0.0020	0.0053	0.0102	0.0159	0.0211	0.0249	0.0266	0.0264
3	0.0016	0.0065	0.0148	0.0245	0.0326	0.0370	0.0371	0.0337	0.0283
4	0.0044	0.0157	0.0301	0.0412	0.0448	0.0406	0.0316	0.0216	0.0130
5	0.0103	0.0302	0.0471	0.0508	0.0416	0.0264	0.0126	0.0039	0.0004
6	0.0204	0.0480	0.0578	0.0452	0.0235	0.0067	0.0002	0.0014	0.0055
7	0.0350	0.0636	0.0550	0.0259	0.0045	0.0004	0.0067	0.0138	0.0169
8	0.0530	0.0707	0.0381	0.0061	0.0011	0.0121	0.0210	0.0212	0.0156
9	0.0722	0.0653	0.0160	0.0004	0.0147	0.0261	0.0228	0.0124	0.0039
10	0.0895	0.0485	0.0015	0.0120	0.0297	0.0248	0.0099	0.0009	0.0008

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$\text{Mn}_2$

$\text{Mn}_2$

Spectroscopic Constants

Dissociation energy =  $0.22 \pm 0.17$  eV, 5 kcal/mole,  $1750 \text{ cm}^{-1}$  (68.2).

$Mn_2$

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N<sub>2</sub>Methods of Production and Experimental Technique

Absorption (in the vacuum ultraviolet).

Emission from discharge into air, pure N<sub>2</sub>, or N<sub>2</sub> in rare gases, hollow cathode discharge, high voltage arc, afterglow, aurora, laser emission, electron beam emission.

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
Vegard-Kaplan Wilkinson Saun-Benesch Ogawa-Tanaka-Wilkinson	I	$A^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Luminescence	5060-2100	R	2760.8(0, 6)		(71.105, 68.80, 68.75, 65.57, 62.40, 61.38, 59.31, 34.6, 34.5, 32.3)
	II	$B^3\Pi_g \leftarrow X^1\Sigma_g^+$	Absorption	1690-1630	R	1635(0, 0) 1638(1, 0)		(62.42)
	III	$W^3\Delta_u \leftarrow X^1\Sigma_g^+$	Absorption	4400-2400				(71.101)
	IV	$B'^3\Sigma_u^- \leftarrow X^1\Sigma_g^+$	Absorption	2240-1120	R			(65.51, 64.46)

Molecule N<sub>2</sub>

N<sub>2</sub>

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
Orlawa-Tanaka-Wilkinson-Mulliken Lyman-Birge-Hopfield Tanaka Tanaka	V	$a^1\Sigma_u^- \rightleftharpoons X^1\Sigma_g^+$	Absorption: N <sub>2</sub> + Ar	2000-1080	R			(66.62, 65.54, 64.46, 60.35, 59.32, 59.30)
	V1	$a^1\Pi_g \rightleftharpoons X^1\Sigma_g^+$	Absorption and discharge	2600-1090	R	2125.0(5, 14) 2041.2(5, 13)		(66.63, 65.59, 65.55, 54.46, 56.25)
	VII	$w^1\Delta_u \rightleftharpoons X^1\Sigma_g^+$	Absorption	1400-1140	R			(64.46)
	VIII	$C^3\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption	1130-1070	R		5 heads	(65.53, 64.46)
	IX	$E^3\Sigma_g^+ \rightleftharpoons X^1\Sigma_g^+$	Energy loss spectra	~ 1050		1043.9(0, 0)		(73.166)

Molecule N<sub>2</sub>

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
Dressler-Lutz	X	$a''^1\Sigma_g^+ \rightleftharpoons X^1\Sigma_g^+$	Absorption	~ 1010		1011.5(0, 0)		(73.166, 67.67)
	XI	$b^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption and discharge	995-855	R	979.5(2, 0)		(73.166, 69.83, 69.82, 69.81, 64.47)
	XII	$F^3\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Energy loss spectra	980-930		972.2(0, 0)		(73.166)
	XIII	$G^3\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Energy loss spectra	970-940		967.7(0, 0)		(73.166)
	XIV	$D^3\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	Energy loss spectra	~ 960		965.4(0, 0)		(73.166)
	XV	$b^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	Absorption and discharge	965-830	R			(69.83, 69.82, 69.81, 64.47)
	XVI	$c^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption and discharge	960-865	R			(69.83, 69.82, 69.81, 64.47)
	XVII	$c^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	Absorption and discharge	960-840	R			(69.83, 69.82, 69.81, 64.47)

Molecule N<sub>2</sub>

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
First Positive Herman-Kaplan Wu-Benesch "YI Bands	XVII	$e^1\Pi_u \approx X^1\Sigma_g^+$	Absorption and discharge	950-880	R			(69.83, 69.82, 69.81, 64.47)
	XIX	$e^1\Pi_u \leftarrow X^1\Sigma_g^+$	Energy loss spectra	~ 860		865.1(0, 0)		(69.90)
	XX	$e^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Energy loss spectra	~ 860		863.8(0, 0)		(69.90)
	XXI	$B^3\Pi_g \rightarrow A^3\Sigma_u^+$	Positive column	Infrared - 4700	V	10510.1(0, 0) 8912.4(1, 0)		(61.38, 59.33)
	XXII	$E^3\Sigma_g^+ \rightarrow A^3\Sigma_u^+$	Luminescence	2740-2130	V	2471.4(0, 4) 2391.1(0, 3)	Bands not resolved	(45.16, 35.9)
	XXIII	$W^3\Delta_u \approx B^3\Pi_g$	Discharge	69000-7000			Bands not resolved	(71.101, 68.73)
	XXIV	$B^3\Sigma_u^- \rightarrow B^3\Pi_g$	Luminescence from discharge	8920-6060	R		Complex structure	(64.45, 60.36, 60.34, 58.29)

Molecule N<sub>2</sub>

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
Second Positive Goldstein-Kaplan Fourth Positive MacFarlane Infrared Fifth Positive	XXV	$C^3\Pi_u \rightarrow B^3\Pi_g$	Positive column	5450-2680	V	3371.3(0, 0) 3576.9(0, 1)		(65.56, 64.49, 60.37, 59.33)
	XXVI	$C^3\Pi_u \rightarrow B^3\Pi_g$	Luminescence	5060-2860	R	4728.0(0, 11)		(64.45, 63.44, 51.38)
	XXVII	$D^3\Sigma_u^+ \rightarrow B^3\Pi_g$	Luminescence from discharge	2910-2250	V	2448.0(0, 2)	5 heads	(40.11)
	XXVIII	$E^3\Sigma_g^+ \rightarrow B^3\Pi_g$	Electron impact	3180-2740	V	2740(0, 0)		(69.88)
	XXIX	$a^1\Pi_g \rightarrow a^1\Sigma_u^-$	Laser emission	82000-33000				(65.58)
	XXX	$x^1\Sigma_g^- \rightarrow a^1\Sigma_u^-$	Discharge	2850-2030	V	2411.7(1, 4)		(56.26)

Molecule N<sub>2</sub>

N<sub>2</sub>

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
First Kaplan MacFarlane Infrared	XXXI	y <sup>1</sup> $\Pi_g \rightarrow a^1\Sigma_u^-$	Discharge	2470-2070	V	2225.9(0, 1)		(57.28)
	XXXII	w <sup>1</sup> $\Delta_u \rightarrow a^1\Pi_g$	Laser emission	36500				(66.64)
	XXXIII	b <sup>1</sup> $\Pi_u \rightarrow a^1\Pi_g$	Discharge	3420-2740	R			(69.82, 69.81, 57.27)
	XXXIV	b' <sup>1</sup> $\Sigma_u^+ \rightarrow a^1\Pi_g$	Discharge	2500	R			(69.82, 69.81, 57.27)
	XXXV	c <sup>1</sup> $\Pi_u \rightarrow a^1\Pi_g$	Discharge	3010-2220	R, V			(69.82, 69.81, 57.27)
	XXXVI	c' <sup>1</sup> $\Sigma_u^+ \rightarrow a^1\Pi_g$	Discharge	3660-2280	R, V			(69.82, 69.81, 57.27)

Molecule N<sub>2</sub>

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
Gaydon-Herman Second Kaplan Gaydon-Herman Gaydon-Herman Gaydon-Herman Gaydon-Herman	XXXVII	d' <sup>1</sup> ? $\Sigma_u^- \rightarrow a^1\Pi_g$	Discharge	2550-2350				(69.82, 69.81, 57.27)
	XXXVIII	b <sup>1</sup> $\Pi_u \rightarrow a^1\Pi_g$	Discharge	2860-2720	R			(69.82, 69.81, 57.27)
	XXXIX	y <sup>1</sup> $\Pi_g \rightarrow w^1\Delta_u$	Discharge	2860-2260	V	2536.6(0, 2)		(57.28)
	XL	z <sup>1</sup> $\Delta_g \rightarrow w^1\Delta_u$	Discharge	2480-2360	V			(57.27)
	XLI	E <sup>3</sup> $\Sigma_g^+ \rightarrow C^3\Pi_u$	Electron impact	12850	V	12843.6(0, 0)	One band observed	(69.88)
	XLII	?	Discharge	6340-5040	V	5815(0, 1)	Bands not resolved	(54.23, 53.22, 44.15)
	XLIII	?	Discharge	8550-7000	V	8057(0, 0)		(53.22, 51.18)

Molecule N<sub>2</sub>

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
Worley-Jenkins	XLIV	$X^2\Sigma_g^+ - X^1\Sigma_g^+$ (N <sub>2</sub> <sup>+</sup> )	Absorption	< 960			Rydberg series	(69.82, 69.81, 67.66, 62.39, 53.21, 53.20, 43.14, 42.13)
Carroll-Yoshino	XLV	$X^2\Sigma_g^+ - X^1\Sigma_g^+$ (N <sub>2</sub> <sup>+</sup> )	Absorption				Rydberg series	(69.82, 69.81, 67.66)
Worley	XLVI	$A^2\Pi_u - X^1\Sigma_g^+$ (N <sub>2</sub> <sup>+</sup> )	Absorption	< 960			Rydberg series	(62.39, 53.21, 53.20)
Hopfield	XLVII	$B^3\Sigma_u^+ - X^1\Sigma_g^+$ (N <sub>2</sub> <sup>+</sup> )	Absorption	< 960			Rydberg series	(62.39, 43.14, 42.13, 38.10, 34.9, 30.1)
	XLVIII	$C^2\Sigma_u^+ - X^1\Sigma_g^+$ (N <sub>2</sub> <sup>+</sup> )	Absorption	570-470			Rydberg series	(66.60, 52.19)
	XLIX	Continuum	Absorption	1000-610				(73.151)

Molecule N<sub>2</sub>

I.  $A^3\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$  (Vegard-Kaplan) System

Band heads,  $\lambda$  (61.38, 50.17):

$v', v''$	2	3	4	5	6	7	8	9
0	2215.1	2332.8	2461.6	2603.6	2760.8	2935.7		3351.5
1	2146.6	2257.2	2377.5	2509.8	2655.5	2817.1	2997.0	3197.5
2		2187.8	2300.7	2424.2	2560.1	2710.1		
3		2123.5	2229.9	2346.0	2472.5	2612.8	2766.9	
4			2164.5	2274.0		2523.4	2666.6	
5				2207.2	2319.7	2441.8	2576.0	2722.5

II.  $B^3\Pi_g^- \leftarrow X^1\Sigma_g^+$  (Wilkinson) System

Band heads:  $(v', v'')$       (0,0)      (1,0)  
 $\lambda$                   1685          1638

III.  $W^3\Delta_u^- \leftarrow X^1\Sigma_g^+$  (Saum-Benesch) System

Band heads,  $\lambda$  (70.101, 70.94):

$v', v''$	0	1	2	3	4	5	6	7	8
0	1683.6	1752.4	1826.0	1905.1	1990.2	2082.0	2181.4	2289.1	2406.4
1	1642.7	1708.1	1778.0	1852.9	1933.3	2019.9	2113.2	2214.2	2323.8
2	1604.4	1666.7	1733.2	1804.3	1880.4	1962.2	2050.2	2145.1	2247.7
3	1568.3	1627.8	1691.2	1758.8	1831.1	1908.5	1991.7	2081.1	2177.6
4	1534.4	1591.3	1651.8	1716.3	1785.0	1858.6	1937.3	2021.9	2112.8
5	1502.9	1557.0	1614.9	1676.4	1742.0	1811.9	1886.7	1966.8	2052.7
6	1472.8	1524.6	1580.1	1639.0	1701.6	1768.3	1839.4	1915.4	1996.9
7	1444.2	1494.1	1547.4	1603.8	1663.7	1727.4	1795.2	1867.5	1944.9
8	1416.9	1465.3	1516.5	1570.6	1628.0	1689.0	1753.7	1822.7	1896.3
9	1391.5	1438.1	1487.3	1539.4	1594.5	1652.9	1714.9	1780.8	1851.0
10	1367.3	1412.3	1459.8	1509.9	1562.8	1618.9	1678.3	1741.4	1808.5

IV.  $B' ^3\Sigma_u^- \leftarrow X ^1\Sigma_g^+$  (Ogawa-Tanaka-Wilkinson) System

Band heads,  $\lambda$  (66.61, 60.35, 59.30):

$v', v''$	0	1	2	3	4	5	6	7	8
0	1518.1			1695.6	1762.6	1834.2		1993.0	2081.2
1	1484.4		1593.9	1653.8	1717.5			1935.4	2018.6
2	1452.8						1808.6	1881.9	
3	1422.9								
4	1394.7								
5	1368.1								
6	1342.8								
7	1318.9								
8	1296.2								
9	1274.7								
10	1254.2								

V.  $a' ^1\Sigma_u^- \rightleftharpoons X ^1\Sigma_g^+$  (Ogawa-Tanaka-Wilkinson-Mulliken) System

Band heads in absorption,  $\lambda$  (Intensity) (66.61):

( $v', v''$ )	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(5, 0)	(6, 0)
(Intensity)	1477.1 (2)	1446.5 (4)	1414.7 (8)	1387.6 (16)	1360.5 (22)	1335.0 (30)	1310.7 (30)
( $v', v''$ )	(7, 0)	(8, 0)	(9, 0)	(10, 0)	(11, 0)	(12, 0)	(13, 0)
(Intensity)	1287.7 (52)	1265.8 (60)	1245.0 (48)	1225.3 (42)	1206.4 (33)	1188.5 (34)	1171.3 (28)
( $v', v''$ )	(14, 0)	(15, 0)	(16, 0)	(17, 0)	(18, 0)	(19, 0)	
(Intensity)	1155.0 (24)	1139.3 (20)	1124.6 (16)	1110.0 (10)	1096.3 (6)	1083.2 (4)	

Band heads in emission,  $\lambda$  (Intensity) (60.33, 59.33):

( $v', v''$ )	(0, 8)	(0, 7)	(0, 6)	(0, 5)	(0, 4)	(0, 3)
(Intensity)	2004.2 (1)	1922.2 (2)	1845.6 (3)	1774.0 (4)	1707.0 (4)	1643.8 (3)

VI.  $a^1\Pi_g \leftarrow X^1\Sigma_g^+$  (Lyman-Birge-Hopfield) System

Band heads in emission,  $\lambda$  (66.61):

$v', v''$	9	10	11	12	13	14	15	16	17
0									
1	1972.6								
2		1988.9	2073.0						
3			2006.0	2089.7	2181.1	2278.3			
4				1944.3	2023.5	2108.1	2198.7	2296.1	
5					1961.8	2041.2	2125.9	2216.6	2314.0
6						1979.5	2059.0	2144.0	2234.8
7									2332.2
									2253.4

VII.  $w^1\Delta_u \leftarrow X^1\Sigma_g^+$  (Tanaka) System

Band heads,  $\lambda$  (Intensity) (64.46):

$(v', v'')$	$(0, 0)$	$(1, 0)$	$(2, 0)$	$(3, 0)$	$(4, 0)$	$(5, 0)$
$\lambda$	1393.9	1364.7	1337.1	1311.0	1286.3	1262.9
(Intensity)		(1)	(2)	(3)	(3)	(4)
$(v', v'')$	$(6, 0)$	$(7, 0)$	$(8, 0)$	$(9, 0)$	$(10, 0)$	$(11, 0)$
$\lambda$	1240.6	1219.4	1199.3	1180.3	1162.1	1144.7
(Intensity)	(5)	(7)	(6)	(6)	(5)	(4)

VIII.  $C^3\Pi_u \leftarrow X^1\Sigma_g^+$  (Tanaka) System

Band heads,  $\lambda$  (Intensity) (66.61):

$(v', v'')$	$(0, 0)$	$(1, 0)$	$(2, 0)$
$\lambda$	1124.2	1099.6	1076.3
(Intensity)	(45)	(60)	(30)

IX.  $E^3\Sigma_g^+ \leftarrow X^1\Sigma_g^+$  System

Represents a part of a Rydberg series corresponding to a N<sub>2</sub><sup>+</sup> X<sup>2</sup>g<sup>+</sup> core.

Band heads,  $\lambda$  (74.188, 73.166):

$(v', v'')$	$(0, 0)$	$(1, 0)$	$(2, 0)$
$\lambda$	1043.9	1020.7	998.9

X.  $a''^1\Sigma_g^+ \leftarrow X^1\Sigma_g^+$  (Dressler-Lutz) System

Represents part of a Rydberg series corresponding to a  $N_2^+ X^2\Sigma_g^+$  core.

Band heads,  $\lambda$  (67.67):

$(v', v'')$	$(0, 0)$	$(1, 0)$
$\lambda$	1011.5	990.9

XI.  $b^1\Pi_u \approx X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (73.166, 69.83, 69.82, 69.81):

$(v', v'')$	$\lambda$	$(v', v'')$	$\lambda$
(0, 0)	991.9	(8, 0)	935.1
(1, 0)	985.6	(9, 0)	929.0
(2, 0)	978.9	(10, 0)	922.7
(3, 0)	972.1	(11, 0)	916.4
(4, 0)	965.7	(12, 0)	910.5
(5, 0)	955.1	(13, 0)	904.7
(6, 0)	949.2	(14, 0)	899.2
(7, 0)	942.4	(15, 0)	895.9

XII.  $F^3\Pi_u \leftarrow X^1\Sigma_g^+$  System

Represents a part of a Rydberg series corresponding to a  $N_2^+ A^2\Pi_u$  core.

Band heads,  $\lambda$  (73.166):

$(v', v'')$	$(0, 0)$	$(1, 0)$	$(2, 0)$
$\lambda$	972.2	955.0	938.4

XIII.  $G^3\Pi_u^- \leftarrow X^1\Sigma_g^+$  System

Represents part of a Rydberg series corresponding to a  $N_2^+ X^2\Sigma_g^+$  core.

Band heads, $\lambda$ (73.166):	(v', v'')	(0, 0)	(1, 0)
	$\lambda$	967.7	949.2

XIV.  $D^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+$  System

Represents part of a Rydberg series corresponding to a  $N_2^+ X^2\Sigma_g^+$  core.

Band head, $\lambda$ (73.166):	(v', v'')	(0, 0)
	$\lambda$	965.4

XV.  $b'^1\Sigma_u^+ \approx X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (69.83, 69.82, 69.81, 64.47):

(v', v'')	$\lambda$	(v', v'')	$\lambda$
(0, 0)	964.6	(8, 0)	-
(1, 0)	957.7	(9, 0)	907.5
(2, 0)	951.0	(10, 0)	901.4
(3, 0)	944.6	(11, 0)	896.2
(4, 0)	937.9	(12, 0)	891.0
(5, 0)	931.9	(13, 0)	885.7
(6, 0)	926.1	(14, 0)	880.7
(7, 0)	917.8	(15, 0)	875.9

XVI.  $c^1\Pi_u^- \approx X^1\Sigma_g^+$  System

$c_3$  represents the first member of a Rydberg series corresponding to a  $N_2^+ X^2\Sigma_g^+$  core.

Band heads, $\lambda$ (69.83, 69.82, 69.81, 64.47):	(v', v'')	$\lambda$
	(0, 0)	960.3
	(1, 0)	920.0

XVII.  $c' \overset{+}{\Sigma}_u^+ \approx X \overset{+}{\Sigma}_g^+$  System

$c'_4$  represents the first member of a Rydberg series corresponding to a  $N_2^+ X \overset{+}{\Sigma}_g^+$  core.

Band heads,  $\lambda$  (69.83, 69.82, 69.81, 64.47):

(v', v'')	$\lambda$	(v', v'')	$\lambda$
(0, 0)	958.6	(4, 0)	886.8
(1, 0)	940.1	(5, 0)	870.8
(2, 0)	921.2	(6, 0)	856.0
(3, 0)	903.7	(7, 0)	841.9

XVIII.  $o' \overset{+}{\Pi}_u \approx X \overset{+}{\Sigma}_g^+$  System

Represents the first member of the Worley Rydberg series corresponding to a  $N_2^+ A \overset{+}{\Pi}_u$  core.

Band heads,  $\lambda$  (69.83, 69.82, 69.81, 64.47):

(v', v'')	$\lambda$
(0, 0)	946.1
(1, 0)	928.9
(2, 0)	912.6
(3, 0)	897.2
(4, 0)	882.5

XIX.  $e' \overset{+}{\Pi}_u \leftarrow X \overset{+}{\Sigma}_g^+$  System

$e'_4$  represents a member of the Worley-Jenkins Rydberg series corresponding to a  $N_2^+ X \overset{+}{\Sigma}_g^+$  core.

Band heads,  $\lambda$  (69.90):

(v', v'')	(0, 0)	(1, 0)	(2, 0)
$\lambda$	865.1	849.9	834.2

XX.  $e' \overset{+}{\Sigma}_u^+ \leftarrow X \overset{+}{\Sigma}_g^+$  System

$e'_4$  represents a member of the Worley-Jenkins Rydberg series corresponding to a  $N_2^+ X \overset{+}{\Sigma}_g^+$  core.

Band head,  $\lambda$  (69.90): (v', v'') (0, 0)  
 $\lambda$  863.8

XXI.  $B^3\Pi_g \rightarrow A^3\Sigma_u^+$  (First Positive) System

Band heads,  $\lambda$  (Intensity) (50.17):

$v', v''$	0	1	2	3	4	5	6
0	10510.0(10)						
1	8912.4(10)						
2	7753.2(6)	8722.3(8)	9942.0(2)				
3	6875.0(2)	7626.2(7)	8541.8(6)	9682.1(3)			
4	6186.8(3)	6788.6(6)	7503.9(7)	8369.2(2)	9436.4(3)		
5	5632.7(1)	6127.4(3)	6704.8(8)	7386.6(5)	8204.8(3)	9203.9(2)	
6		5592.9(1)	6069.7(7)	6623.6(9)	7273.3(3)	8047.4(2)	
7			5553.7(1)	6013.6(7)	6544.8(10)	7164.8(2)	7896.4(2)
8				5515.6(2)	5959.0(8)	6468.5(10)	7059.0(2)
9					5478.5(2)	5906.0(8)	6394.7(9)
10						5442.3(3)	5854.4(8)
11						5053.6	5407.1(3)
12							5030.8

XXII.  $E^3\Sigma_g^+ \rightarrow A^3\Sigma_u^+$  (Herman-Kaplan) System

Band heads,  $\lambda$  (74.188, 45.16, 35.9):

$v', v''$	0	1	2	3	4	5	6	7
0		2242.3	2315.3	2391.6	2471.4	2554.9	2642.1	2733.2
1		2137.6	2203.8	2272.9		2419.8	2497.8	

XXIII.  $W^3\Delta_u \rightleftharpoons B^3\Pi_g$  (Wu-Benesch) System

Band heads,  $\lambda$  (n.p. 218, 71.101, 70.92, 68.73):

$v', v''$	0	1	2	3	4	5	6
0	629373.3	-65875.5	-31578.9	-20889.5	-15675.8	-12589.4	-10549.8
1	61962.2	586939.5	-58422.4	-30011.2	-20307.6	-15412.6	-12462.8
2	32833.3	73057.5	-357305.2	-52623.6	-28633.1	-19777.0	-15169.8
3	22450.3	36005.1	88595.4	-203381.4	-47987.9	-27413.9	-19292.1
4	17124.2	24002.4	39775.2	111892.7	-143172.7	-44201.2	-26329.2
5	13885.3	18099.6	25797.6	44328.0	150660.7	-111088.6	-41053.2
6	11708.4	14568.8	19174.3	27817.1	49931.5	227885.3	-91169.0
7	10145.4	12225.3	15311.3	20363.6	30133.7	56992.5	456755.3
8	8969.2	10557.0	12781.6	16120.4	21686.6	32816.8	66157.9
9	8052.4	9309.4	10997.3	13382.0	17005.2	23166.3	35959.1
10	7318.0	8341.7	9671.8	11469.3	14051.7	17976.5	24831.6

XXIV.  $B' ^3\Sigma_u^- \rightarrow B ^3\Pi_g$  ("Y" Bands) System

Band heads,  $\lambda$  (Intensity) (50.17):

$v', v''$	0	1	2	3	4
4	8058(2)				
5	7243(2)	8262(5)			
6	6587(1)	7420(6)	8473(8)		
7	6062(1)	6744(6)	7602(10)	8691(10)	
8		6203(3)	6905(10)	7791(10)	8917(2)

XXV.  $C ^3\Pi_u \rightarrow B ^3\Pi_g$  (Second Positive) System

Band heads,  $\lambda$  (Intensity) (50.17):

$v', v''$	0	1	2	3	4	5
0	3371.3(10)	3576.9(10)	3804.9(10)	4059.4(8)	4343.6(4)	4667.3(0)
1	3159.3(9)	3338.9(2)	3536.7(8)	3755.4(10)	3998.4(9)	4269.7(5)
2	2976.8(6)	3136.0(8)	3309(2)	3500.5(4)	3710.5(8)	3943.0(8)
3	2819.8(1)	2962.0(6)	3116.7(6)	3285.3(3)	3469(0)	3671.9(6)
4	2687	2814.3(1)	2953.2(6)	3104.0(3)	3268.1(4)	3446(0)

XXVI.  $C' ^3\Pi_u \rightarrow B ^3\Pi_g$  (Goldstein-Kaplan) System

Band heads,  $\lambda$  (50.17):

$v', v''$	2	3	4	5	6	7	8	9	10
0	2863.5	3005.4	3159.2	3326.1	3504.0	3707.1	3925.4	4166.0	4432.2
1			3025.8	3178.4					

XXVII.  $D ^3\Sigma_u^+ \rightarrow B ^3\Pi_g$  (Fourth Positive) System

Band heads,  $\lambda$  (Intensity) (50.17):

$(v', v'')$	(0, 6)	(0, 5)	(0, 4)	(0, 3)	(0, 2)	(0, 1)	(0, 0)
$\lambda$	2903.9	2777.9	2660.5	2550.7	2448.0	2351.4	2260.8
(Intensity)	(1)	(2)	(5)	(8)	(10)	(6)	(2)

N<sub>2</sub>

XXVIII. E<sup>3Σ<sup>+</sup> → B<sup>3Π<sub>g</sub> System</sup></sup>

Band heads, λ (69.88):

(v', v'')	(0,0)	(0,1)	(0,2)	(0,3)
λ	2740	2880	3020	3180

XXIX. a<sup>1Π<sub>g</sub> → a'<sup>1Σ<sup>-</sup> (MacFarlane Infrared) System</sup></sup>

Band heads, λ (65.58):	(v', v'')	(0,0)	(1,0)	(2,1)
λ	82489.2	34739.4	33214.5	

XXX. x<sup>1Σ<sup>-</sup> → a'<sup>1Σ<sup>-</sup> (Fifth Positive) System</sup></sup>

Band heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4	5	6
0	2198.9(4)	2274.3(6)	2353.6(4)		2525.6(2)	2619.3(4)	
1	2112.1(5)	2181.5(4)		2331.3(2)	2411.8(7)	2496.7(3)	2586.6(7)
2	2033.6(5)	2097.9(2)	2165.2(5)	2235.9(3)		2387.9	2469.9(4)

XXXI. y<sup>1Π<sub>g</sub> → a'<sup>1Σ<sup>-</sup> (First Kaplan) System</sup></sup>

Band heads, λ (Intensity) (50.17):

v', v''	0	1	2	3	4
0	2153.6(4)	2225.9(5)	2301.9(4)	2381.7(3)	2466.0(2)
1	2077.3			2288.6(1)	2366.4(2)

XXXII. w<sup>1Δ<sub>u</sub> → a'<sup>1Π<sub>g</sub> (MacFarlane Infrared) System</sup></sup>

Band head, λ (66.64):	(v', v'')	(0,0)
λ		36399.5

XXXIII.  $b^1\Pi_u \rightarrow a^1\Pi_g$  (Gaydon-Herman) System

Band heads,  $\lambda$  (69.82, 69.81, 57.27):

$v', v''$	0	1	2	3	4
0					
1	3075.1	3241.3			
...					
5	2795.4	2932.0	3079.9	3240.8	3416.5
6	2746.2	2877.9	3020.3	3175.0	

XXXIV.  $b^1\Sigma_g^+ \rightarrow a^1\Pi_g$  (Gaydon-Herman) System

Band head,  $\lambda$  (69.82, 69.81, 57.27):  $(v', v'')$   $\lambda$  (0, 7)  
2498.6

XXXV.  $c^1\Pi_u \rightarrow a^1\Pi_g$  (Gaydon-Herman) System

$c_3$  and  $c_4$  are the two first members of a  $c^1\Pi_u$  Rydberg series  
that converges at  $N_2^+ X^2\Sigma_g^+$ .

Band heads,  $\lambda$  (69.82, 69.81, 57.27):

$c_3^1\Pi_u \rightarrow a^1\Pi_g$

$v', v''$	0	1	2	3	4
0	2839.4	2980.1			
1					
2	2516.0	2626.2	2744.3	2871.1	3008.1

$c_4^1\Pi_u \rightarrow a^1\Pi_g$

$v', v''$	0	1	2	3	4	5	6
0		2224.4	2308.6	2397.8	2492.4	2592.8	2699.9

XXXVI.  $c' \overset{+}{\Sigma}_{u}^{\circ} \rightarrow a \overset{+}{\Pi}_{g}$  (Gaydon-Herman) System

$c'_4$  is the first member of a  $c' \overset{+}{\Sigma}_{u}^{\circ}$  Rydberg series that converges at  $N_2^+ X^2 \overset{+}{\Sigma}_{g}$ .

Band heads,  $\lambda$  (69.82, 69.81, 57.27):

$v', v''$	0	1	2	3	4	5
0	2827.1	2967.0	3118.6	3283.3	3463.3	3661.1
1	2671.7	2796.0				
2	2524.9		2753.8			
3	2397.1	2496.8	2603.3			
4	2281.5	2371.6	2467.7	2569.6	2678.5	2795.6

XXXVII.  $d'(\overset{-}{\Sigma}_{u}^{\circ} \text{ or } \overset{+}{\Delta}_{u}) \rightarrow a \overset{+}{\Pi}_{g}$  (Gaydon-Herman) System

Band heads,  $\lambda$  (69.82, 69.81, 57.27):

$v', v''$	0	1	2
0	2358.8	2455.1	2558

XXXVIII.  $o \overset{+}{\Pi}_{u} \rightarrow a \overset{+}{\Pi}_{g}$  (Gaydon-Herman) System

$o$  is the first member of the Worley Rydberg series that converges at  $N_2^+ A^2 \overset{+}{\Pi}_{u}$ .

Band heads,  $\lambda$  (69.82, 69.81, 57.27):  $(v', v'')$   $\lambda$  (0, 0) 2723.6 (0, 1) 2853.3

XXXIX.  $y \overset{+}{\Pi}_{g} \rightarrow w \overset{+}{\Delta}_{u}$  (Second Kaplan) System

Band heads,  $\lambda$  (Intensity) (50.17):

$v', v''$	0	1	2	3	4	5	6
0	2354.5(4)		2536.6(5)	2636.2(5)	2741.9(3)	2854.9	
1	2263.4(4)		2431.0	2522.3(3)	2619.3(5)	2722.0(3)	2831.7

XL.  $z^1\Delta_g \rightarrow w^1\Delta_u$  System

Band heads,  $\lambda$  (57.27):  $(v', v'')$   $\lambda$  (n, 2) 2477.3 (n+3, 4) 2368.8 for n = 2?

XLI.  $E^3\Sigma_g^+ \rightarrow C^3\Pi_u$  System

Band head,  $\lambda$  (69.88):  $(v', v'')$   $\lambda$  (0, 0) 12843.6

XLII. Gaydon Green System

Band heads,  $\lambda$  (54.23, 53.22, 44.15):

$v', v''$	0	1	2	3	4	5
0	5574.4(9)	5815.1(10)	6068.6(8)	6336.3(5)		
1	5308.6(8)	5527.1(2)	5755.1(3)	5994.5(6)	6246.3(5)	
2	5073.4(4)	5272.0(5)	5479.6(6)		5924 (1)	6160.5(3)
3		5047.0(2)		5435.0(3)	5640 (1)	

XLIII. Herman Infrared System

Band heads,  $\lambda$  (53.22, 51.18):

$v', v''$	0	1	2
0	8057.6(10)	8549 (2)	
1	7521.0(0)		8397 (1)
2	7061.7(6)	7435.0(5)	7828.5(8)
3		7001.2(4)	

XLIV.  $X^2\Sigma_g^+(N_2^+)$  -  $X^1\Sigma_g^+$  (Worley-Jenkins) System

Represents a  $^1\Pi_u$  Rydberg series, the first state of which is  $c^1\Pi_u$  (69.82, 69.81, 67.66, 62.39)

$$\nu = 125665.8 - R \left[ m + 0.3450 - (0.1000/m) - (0.100/m^2) \right]^{-2}$$

where  $m = 2, 3, \dots, 26$

XLV.  $X^2\Sigma_g^+(N_2^+) \leftarrow X^1\Sigma_g^+$  (Carroll-Yoshino) System

Represents a  $^1\Sigma_u^+$  Rydberg series, the first member of which is  
 $c' ^1\Sigma_u^+$  (69.82, 69.81, 67.66)

m	2	3	4	5	6	7
$\lambda$	958.559	(863.6)	833.746	820.592	(813.2)	808.672
n*	2.2675		4.3776	5.3713		7.394

XLVI.  $A^2\Pi_u(N_2^+) \leftarrow X^1\Sigma_g^+$  (Worley) System

Represents a  $^1\Pi_u$  Rydberg series, the first of which is  $o ^1\Pi_u$  (62.39, 53.21, 53.20)

$$v = 136607 - R \left[ m - 0.0441 - (0.018/m^2) \right]^{-2} \text{ where } m = 2, 3, \dots 6$$

XLVII.  $B^2\Sigma_u^+(N_2^+) \leftarrow X^1\Sigma_g^+$  (Hopfield) System

Represents a Rydberg series (62.39, 43.14, 42.13, 38.10, 24.8, 30.1)

$$v = 151240 - R(m - 0.092)^{-2} \text{ where } m = 3, 4, \dots 7$$

XLVIII.  $C^2\Sigma_u^+(N_2^+) \leftarrow X^1\Sigma_g^+$  System

Represents a Rydberg series

Band heads,  $\lambda$  (66.60, 52.19):

$n^* = 3.040$	$(v', v'')$	$\lambda$	$(v', v'')$	$\lambda$
	(0, 0)	560.48	(7, 0)	520.46
	(1, 0)	554.10	(8, 0)	515.61
	(2, 0)	548.00	(9, 0)	510.93
	(3, 0)	542.11	(10, 0)	506.35
	(4, 0)	536.41	(11, 0)	502.02
	(5, 0)	530.86	(12, 0)	497.77
	(6, 0)	525.54	(13, 0)	493.71

n* = 4.059	(v', v'')	λ
	(3, 0)	527. 33
	(4, 0)	521. 89
	(5, 0)	516. 71
	(6, 0)	
	(7, 0)	506. 71
	(8, 0)	502. 02

n* = 5.05	(v', v'')	λ
	(8, 1)	496. 15

XLIX. Continuum

There are two weak continua between 825 and 1000 Å with maximums of approximately  $5 \text{ cm}^{-1}$  at 970 Å and  $15 \text{ cm}^{-1}$  at 910 Å. At approximately 850 Å a dissociation continuum increases gradually to a maximum of  $\sim 120 \text{ cm}^{-1}$  at 805 Å. This is followed by a secondary peak with a maximum value of  $75 \text{ cm}^{-1}$  occurring at 775 Å. The continuum then decreases to 0 at  $\sim 750 \text{ Å}$ . The most prominent dissociation continuum starts at approximately 730 Å and decreases to  $90 \text{ cm}^{-1}$  at 660 Å. Below 660 Å there is another continuum with a broad maximum at 610 Å, this continuum overlapping the previous one. (73.151)

SPECTROSCOPIC CONSTANTS

Molecule  $N_2$

State	$T_o$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$e' 1\Sigma_u^+$	115767.5							Rydberg	(69.90)
$e 1\Pi_u$	115593.6							Rydberg	(69.90)
$z 1\Delta_g$	115365.9	(1700)		(1.76)	15.3			Rydberg	(57.27)
$y 1\Pi_g$	114166.3	1707.9 <sup>(a)</sup>		1.78(b)			1.16(c)	Rydberg	(57.28)
$x 1\Sigma_g^-$	113212.1	1910.0		1.750	22.5	5.88	1.168	Rydberg	(56.26)
$d' 1\Pi_u$	111333								(45.16)
$o 1\Pi_u$	105682	2020.0	32.28	1.694(b)			1.19(c)	Rydberg	(69.82, 69.81)
$c' 1\Sigma_u^+$	104322.4	2046(a)		1.929(b)			1.12(c)	Rydberg	(69.82, 69.81)
$c' \Pi_u$	10439.2	2410(a)		1.50(b)			1.27(c)	Rydberg	(69.82, 69.81)
$b' 1\Sigma_u^+$	103672	746(a)		1.154	4.8		1.444		(69.82, 69.81)
$D 3\Sigma_u^+$	103573			1.961(b)		20	1.108 <sup>(c)</sup>	Rydberg	(40.11)

## SPECTROSCOPIC CONSTANTS

State	$T_o$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$G^3\Pi_u$	103338							Rydberg	(73.166)
$F^3\Pi_u$	102854							Rydberg	(73.166)
$b^1\Pi_u$	100816	635 (a)		1.448 (b)	4.8	29			
$a''^1\Sigma_g^+$	99032								(69.86, 69.81)
$C'^3\Pi_u$	97580			1.0496 (b)					(67.67)
$E^3\Sigma_g^+$	95774.50	2185 (a)		1.927 (b)					(63.44)
$C^3\Pi_u$	88977.9	2047.18	28.4450	1.82473	18.683	5.80	1.1487	Rydberg	(74.188, 54.50)
$5\Sigma^-$	77925	650					0.0011	1.55	(65.50)
w $^1\Delta_u$	71698.8	1559.24	11.8874	1.498	16.6		5.53	1.2678	(62.41)
$a^1\Pi_g$	68951.2	1694.20	13.9491	1.61688	17.933	5.89		1.2203	(65.50)
$a'^1\Sigma_u^-$	67739.3	1530.25	12.0747	1.47988	16.574	5.54		1.2755	(65.50)

## SPECTROSCOPIC CONSTANTS

State	T <sub>o</sub>	$\omega_e$	$x_e \omega_e$	B <sub>e</sub>	$\alpha_e \times 10^3$	D <sub>e</sub> $\times 10^6$	r <sub>e</sub>	Remarks	Bibliography
B' $^3\Sigma_u^-$	65852.4	1516.88	12.1810	1.47359	16.861	5.56	1.2782		(65.50)
W $^3\Delta_u$	60555.8	1501.4	11.6				1.28		(71.101, 65.50)
B $^3\Pi_g$	59306.8	1733.39	14.1221	1.6374	17.91	5.84	1.2126		(65.50)
A $^3\Sigma_u^+$	49754.8	1460.52	13.8313	1.45455	18.009	5.77	1.2866		(65.50)
X $^1\Sigma_g^+$	0	2358.03	14.1351	1.9980	17.72	5.74	1.0977		(65.50)

(a)  $\Delta G_0$ , (b) B<sub>o</sub>, (c) r<sub>o</sub>Dissociation energy = 9.76  $\pm$  0.01 eV, 225.07 kcal/mole, 78710 cm<sup>-1</sup> (63.43, 56.24).

### Perturbations and General Information

The  $D^3\Sigma_u^+$  state is predissociated by the shallow  $C'^3\Pi_u$  state (74.188).

The  $b^1\Pi_u$  state is perturbed by the  $c^1\Pi_u$  state  
 The  $b'^1\Sigma_u^+$  state is perturbed by the  $c'^1\Sigma_u^+$  state } (73.166)

The  $o^1\Pi_u$  level is predissociated possibly by the  $C'^3\Pi_u$  state (73.166).

The  $B^3\Pi_g$  ( $v' \sim 12$ ) and a  $^1\Pi_g$  ( $v' \sim 6$ ) levels are predissociated by the  $^5\Sigma^+$  level (68.80).

The higher levels of the  $C^3\Pi_u$  and  $C'^3\Pi_u$  states are predissociated by the  $^3\Pi_u$  continuum (69.82).

Perturbations and predissociation have been observed in the  $y$  state (57.28).

### Lifetimes:

$A^3\Sigma_u^+$	$v' = 0$	$\tau = 1.36 + 0.27$ sec for $\Sigma = 0$ substate levels (69.L2, 69.L3)
		$\tau = 2.70 \pm 0.54$ sec for $\Sigma = 1, -1$ substate levels

$B^3\Pi_g$	$v' = 0$	$\tau = 10 + 2$ $\mu$ sec	(n.p. 217)
	$v' = 2$	$\tau = 7.0 \pm 0.4$ $\mu$ sec	(66.L1)
	$v' = 3$	$\tau = 6.8 \pm 0.3$ $\mu$ sec	
	$v' = 4$	$\tau = 6.7 \pm 0.7$ $\mu$ sec	
	$v' = 5$	$\tau = 6.7 \pm 1.0$ $\mu$ sec	
	$v' = 6$	$\tau = 7.0 \pm 0.7$ $\mu$ sec	
	$v' = 7$	$\tau = 5.4 \pm 0.8$ $\mu$ sec	
	$v' = 8$	$\tau = 5.4 \pm 0.8$ $\mu$ sec	
	$v' = 9$	$\tau = 5.4 \pm 0.5$ $\mu$ sec	

$w^3\Delta_u$	$v' = 0$	$\tau = 1.668$ msec	(73.167)
	$v' = 1$	$\tau = 2.000$ msec	

$a'^1\Pi_g$	$v' = 0$	$\tau = 0.17$ msec	(65.52)
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$C^3\Pi_u$	$v' = 0$	$\tau = 40.4 + 0.5$ nsec	(73.177)
	$v' = 1$	$\tau = 40.6 \pm 0.5$ nsec	

$D^3\Sigma_u^+$	$v' = 0$	$\tau = 14.1$ nsec	(73.182)
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Oscillator Strengths:

$$A^3\Sigma_u^+ \leftarrow X^1\Sigma_g^+ \quad f_{0,0} = 2 \times 10^{-3} \quad (66.L1)$$

$$a'^\Pi_g \leftarrow X^1\Sigma_g^+ \quad f_{0,0} = 1.3 \times 10^{-6} \quad (67.68)$$

$$f_{1,0} = 3.0 \times 10^{-6}$$

$$f_{2,0} = 4.1 \times 10^{-6}$$

$$C^3\Pi_u \leftarrow X^1\Sigma_g^+ \quad f_{0,0} = 2.2 \times 10^{-6}$$

$$f_{1,0} = 1.1 \times 10^{-6}$$

$$f_{2,0} = 5.6 \times 10^{-7}$$

$$w^1A_u \leftarrow X^1\Sigma_g^+ \quad \left. \begin{array}{l} f_{3,0} = (3.5 + 0.18p) \times 10^{-8} \\ f_{4,0} = (6.1 + 0.21p) \times 10^{-8} \\ f_{5,0} = (4.0 + 0.26p) \times 10^{-8} \end{array} \right\} \text{for pressure } p \text{ in psi}$$

Franck-Condon factors for the  $C^3\Pi_u - B^3\Pi_g$  (Second Positive) system (65.52):

$v''$ , $v'$	0	1	2	3	4
0	4.55-1	3.88-1	1.34-1	2.16-2	1.16-3
1	3.31-1	2.29-2	3.35-1	2.52-1	5.66-2
2	1.45-1	2.12-1	2.30-2	2.04-1	3.26-1
3	4.94-2	2.02-1	6.91-2	8.81-2	1.13-1
4	1.45-2	1.09-1	1.69-1	6.56-3	1.16-1
5	3.87-3	4.43-2	1.41-1	1.02-1	2.45-3
6	9.68-4	1.52-2	7.72-2	1.37-1	4.70-2
7	2.31-4	4.68-3	3.32-2	9.93-2	1.09-1
8	5.36-5	1.33-3	1.23-2	5.26-2	1.04-1
9	1.21-5	3.57-4	4.12-3	2.31-2	6.67-2
10	2.61-6	9.15-5	1.27-3	8.95-3	3.40-2

Franck-Condon factors followed by a factor of ten

Franck-Condon factors for the  $B^3\Pi_g - A^3\Sigma_g^+$  (First Positive) system (65.52):

$v''$ , $v'$	0	1	2	3	4	5	6	7	8
0	4.06-1	4.01-1	1.58-1	3.17-2	3.47-3	2.01-4	5.72-6	8.81-8	8.28-11
1	3.27-1	3.71-3	2.85-1	2.77-1	9.18-2	1.41-2	1.07-3	3.70-5	5.14-7
2	1.64-1	1.59-1	6.59-2	1.05-1	3.06-1	1.63-1	3.41-2	3.26-3	1.35-4
3	6.67-2	1.93-1	2.25-2	1.50-1	1.11-2	2.59-1	2.26-2	6.36-2	7.50-3
4	2.44-2	1.29-1	1.22-1	4.67-3	1.53-1	6.94-3	1.76-1	2.68-1	1.01-1
5	8.38-3	6.57-2	1.39-1	4.09-2	4.94-2	1.00-1	5.05-2	9.30-2	2.83-1
6	2.80-3	2.92-2	9.94-2	1.03-1	2.04-3	9.29-2	4.02-2	9.90-2	3.20-2
7	9.26-4	1.20-2	5.66-2	1.08-1	5.13-2	8.81-3	1.04-1	5.00-3	1.26-1
8	3.07-4	4.73-3	2.83-2	7.88-2	8.85-2	1.22-2	3.92-2	8.29-2	2.75-3
9	1.03-4	1.83-3	1.31-2	4.78-2	8.58-2	5.37-2	4.73-5	6.71-2	4.68-2

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the  $A^3\Sigma_u^+ - X^1\Sigma_g^+$  (Vegard-Kaplan) system (65.52):

$v''$ , $v'$	0	1	2	3	4	5	6	7	8
0	1.06-3	5.55-3	1.57-2	3.15-2	5.07-2	6.93-2	8.38-2	9.21-2	9.38-2
1	8.41-3	3.27-2	6.65-2	9.31-2	9.91-2	8.35-2	5.57-2	2.78-2	8.41-3
2	3.34-2	8.88-2	1.15-1	8.91-2	4.00-2	5.73-3	1.92-3	1.90-2	3.87-2
3	8.29-2	1.33-1	8.12-2	1.35-2	3.65-3	3.44-2	5.52-2	4.64-2	2.21-2
4	1.44-1	1.09-1	9.45-3	1.74-2	6.05-2	5.16-2	1.45-2	1.60-4	1.52-2
5	1.89-1	3.67-2	1.77-2	7.36-2	3.88-2	4.23-4	1.88-2	4.41-2	3.63-2
6	1.92-1	8.43-5	8.13-2	4.21-2	1.05-2	4.10-2	4.70-2	1.23-2	1.06-3
7	1.55-1	4.26-2	7.92-2	1.22-4	5.28-2	4.21-2	8.71-4	1.90-2	4.11-2
8	1.02-1	1.17-1	1.76-2	4.83-2	5.01-2	5.30-5	3.71-2	4.04-2	5.56-3
9	5.47-2	1.53-1	6.52-3	8.10-2	8.41-4	4.56-2	3.70-2	8.28-6	2.58-2
10	2.46-2	1.32-1	7.06-2	3.10-2	3.70-2	4.73-2	5.09-4	4.04-2	3.06-2

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the  $a^1\Pi_g - X^1\Sigma_g^+$  (Lyman-Birge-Hopfield) system (65.52):

$v''$ , $v'$	0	1	2	3	4	5	6
0	4.43-2	1.18-1	1.73-1	1.85-1	1.60-1	1.20-1	8.08-2
1	1.51-1	1.90-1	9.44-2	1.15-2	6.67-3	4.75-2	8.52-2
2	2.50-1	8.02-2	3.30-3	7.51-2	9.62-2	4.70-2	4.94-3
3	2.53-1	5.84-4	1.08-1	6.81-2	4.43-4	3.47-2	7.32-2
4	1.73-1	9.22-2	8.41-2	4.39-3	7.81-2	5.51-2	2.37-3
5	8.61-2	1.91-1	3.19-4	9.76-2	3.47-2	9.80-3	6.39-2
6	3.22-2	1.76-1	7.30-2	6.18-2	2.05-2	7.84-2	1.24-2
7	9.17-3	9.93-2	1.73-1	1.17-3	9.90-2	5.16-3	4.47-2
8	1.99-3	3.87-2	1.60-1	9.17-2	2.93-2	5.50-2	5.01-2
9	3.37-4	1.10-2	8.76-2	1.71-1	1.64-2	8.17-2	5.19-3
10	4.75-5	2.33-3	3.23-2	1.38-1	1.25-1	3.08-3	8.54-2

Franck-Condon factors followed by a factor of ten

N<sub>2</sub>

Franck-Condon factors for the C<sup>3</sup>Π<sub>u</sub> - X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> (Tanaka) system (65.52):

v'', v'	0	1	2	3	4
0	5.50-1	3.03-1	1.01-1	2.76-2	7.16-3
1	3.36-1	8.73-2	2.71-1	1.82-1	7.88-2
2	9.03-2	3.64-1	1.82-3	1.30-1	1.82-1
3	1.33-2	1.95-1	2.44-1	7.11-2	2.42-2
4	1.12-3	4.47-2	2.67-1	9.92-2	1.48-1
5	6.28-5	5.84-3	9.52-2	2.80-1	9.47-3
6	6.12-6	5.13-4	1.80-2	1.58-1	2.19-1
7	6.77-7	4.90-5	2.27-3	4.32-2	2.13-1
8	4.83-9	5.17-6	2.79-4	8.06-3	8.76-2
9	1.44-10	1.48-7	4.21-5	1.39-3	2.40-2
10	1.68-8	9.72-8	4.41-6	2.59-4	5.66-3

Franck-Condon factors followed by factor of ten

Franck-Condon factors for the W<sup>3</sup>Δ<sub>u</sub> - X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> system (70.94):

v', v''	0	1	2	3	4	5	6	7
0	.1713-2	.1310-1	.4721-1	.1065-6	.1691-0	.2005-0	.1845-0	.1354-0
1	.8568-2	.4711-1	.1107-0	.1384-0	.8733-1	.1401-1	.9521-2	.7826-1
2	.2295-1	.8741-1	.1204-0	.5727-1	.1253-3	.4533-1	.9516-1	.5355-1
3	.4383-1	.1099-0	.7206-1	.1040-2	.4385-1	.7576-1	.1548-1	.1425-1
4	.6680-1	.1025-0	.1818-1	.2143-1	.6970-1	.1385-1	.1912-1	.6786-1
5	.8696-1	.7284-1	.7807-4	.5735-1	.3075-1	.7809-2	.5891-1	.1536-1
6	.1003-0	.3743-1	.1649-1	.5698-1	.5108-3	.4486-1	.2615-1	.8806-2
7	.1050-0	.1106-1	.4202-1	.2820-1	.1368-1	.4519-1	.2614-4	.4465-1
8	.1021-0	.3046-3	.5511-1	.4007-2	.3909-1	.1477-1	.2141-1	.3225-1
9	.9325-1	.3737-2	.4992-1	.1816-2	.4350-1	.1630-4	.4062-1	.2814-2
10	.8129-1	.1581-1	.3329-1	.1623-1	.2659-1	.1279-1	.2831-1	.6968-2

Franck-Condon factors followed by a factor of ten

r-Centroids for the B<sup>3</sup>Σ<sub>u</sub><sup>-</sup> - X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> system (66.65a).

v', v''	0	1	2	3	4	5	6	7	8
0	1.182	1.199	1.216	1.234	1.252	1.271	1.290	1.310	1.330
1	1.171	1.188	1.205	1.222	1.240	1.258	1.277	1.296	1.316
2	1.161	1.177	1.194	1.211	1.228	1.246	1.264	1.283	1.302
3	1.151	1.167	1.183	1.200	1.217	1.234	1.252	1.270	1.289

Lasing from the First Positive system has been observed (n.p. 217, 67.68a, 63.43a).

Lasing from the Second Positive system has been observed (n.p. 217, 74.206, 74.204, 74.199, 74.197, 74.195, 74.193, 74.191, 74.190, 74.189, 73.168, 73.165, 73.163, 68.74a, 67.68a, 66.64a, 64.47a).

Lasing from the Lyman-Birge-Hopfield system has been observed (73.168).

The two MacFarlane infrared systems have only been seen in lasing (n.p. 217 66.65, 66.63a, 65.58).

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$\text{Na}_2$

$\text{Na}_2$

Methods of Production and Experimental Technique

Absorption.

Emission from a discharge in  $\text{Na}_2$  vapor, heat pipe.

Fluorescence.

BAND SYSTEMS

System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
I	$A^1\Sigma_u^+ \approx X^1\Sigma_g^+$	Absorption, discharge, fluorescence	8000-6000	R			(70.44, 33.20, 29.13)
II	$B^1\Pi_u \approx X^1\Sigma_g^+$	Absorption, discharge, fluorescence	5040-4560	R			(69.41, 32.17, 28.10)
III	$C^1\Pi_u \approx X^1\Sigma_g^+$	Absorption, discharge	3600-3200	R	3338.8(5, 0) 3326.3(6, 0)		(50.34, 49.33)
IV	$D^1\Pi_u \approx X^1\Sigma_g^+$	Absorption	3325-3030	R			(50.34)
V	$E \approx ?$	Absorption, discharge	3120-2880	R	2945.5(7, 0)		(47.31)
VI	?	Absorption, discharge	3050-2500	R	2750, 2735		(47.31)

Molecule  $\text{Na}_2$

I.  $A^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$  System

Most intense band heads in absorption,  $\lambda$  (33.20, 29.13):

(v', v'')	(4, 2)	(4, 1)	(5, 1)	(6, 0)	(7, 0)	(8, 0)	(9, 0)
$\lambda$	6751.2	6679.7	6561.5	6513.2	6465.8	6418.4	6374.2

II.  $B^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$  System

Most intense band heads in absorption,  $\lambda$  (32.17, 28.10):

(v', v'')	(0, 3)	(0, 2)	(0, 1)	(1, 1)	(0, 0)	(1, 0)	(2, 0)	(3, 0)
$\lambda$	5040.4	5001.4	4962.8	4932.6	4924.2	4894.5	4865.5	4837.2

III.  $C^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$  System

Most intense band heads,  $\lambda$  (absorption intensity, emission intensity) (50.34, 49.3):

(v', v'')	(5, 1)	(4, 0)	(5, 0)	(6, 0)	(7, 0)	(9, 0)	(10, 0)
$\lambda$	3356.5	3351.5	3338.8	3326.3	3314.0	3290.0	3278.4
Absorption intensity	8	7	10	10	10	9	8
Emission intensity	4	4	5	4	4	4	4

IV.  $D^1\Pi_u \leftarrow X^1\Sigma_g^+$  System

Most intense band heads,  $\lambda$  (Intensity) (50.34):

(v', v'')	(1, 2)	(3, 3)	(2, 2)	(1, 1)	(0, 0)	(2, 1)	(1, 0)	(2, 0)
$\lambda$	3151.6	3145.2	3140.0	3135.7	3131.2	3125.1	3120.5	3109.5
(Intensity)	2	2	2	2	2	2	2	2

V. E ≈ ? System

Most intense band heads,  $\lambda$  (absorption intensity, emission intensity)  
(47.31):

$\lambda$	2983.1	2959.6	2945.5	2936.2	2932.5	2928.6	2927.6
Absorption intensity	6	6	10	8	6	6	8
Emission intensity	0	0	0	4	2	2	4

VI. 3050-2500 Å Bands

Possibly four fragmentary systems (4-7), preliminary vibrational analysis,  $\lambda$  (Intensity) (47.31):

$(v', v'')$	(0, 3)	(1, 3)	(0, 1)	(2, 1)	(0, 0)	(1, 0)	(2, 0)	(8, 0)	(0, 6)
$\lambda$	2986.4	2977.0	2958.6	2948.2	2944.0	2935.6	2970.6	2750.0	2735.0
Intensity	6	5	5	6	5	8	5	5	5
System	4	4	4	4	4	4	4	5	6

## SPECTROSCOPIC CONSTANTS

State	T <sub>e</sub>	ω <sub>e</sub>	x <sub>e</sub> ω <sub>e</sub>	B <sub>e</sub>	α <sub>e</sub> × 10 <sup>4</sup>	D <sub>e</sub> × 10 <sup>6</sup>	r <sub>e</sub>	Remarks	Bibliography
D <sup>1</sup> Π <sub>u</sub>	33486.9	111.93	0.573	0.1152	11.0				(60.35)
C <sup>1</sup> Π <sub>u</sub>	29384.8	119.53	0.782	0.1185	9.6				(60.35, 32.17)
B <sup>1</sup> Π <sub>u</sub>	20319.596	124.065	0.6863	0.125829	8.6754	0.3614	3.41398	(a)	(69.41, 32.17)
A <sup>1</sup> Σ <sub>u</sub> <sup>+</sup>	14680.4	117.6	0.38	0.1107	5.4		3.64		(29.13)
bΠ(0 <sup>+</sup> <sub>u</sub> ) (b)	<14680.4	~145		~0.14					(33.21)
X <sup>1</sup> Σ <sub>g</sub> <sup>+</sup>	0	159.126	0.7262	0.154853	8.5637	0.6552	3.07745	(c)	(69.41, 33.20)

(a) y<sub>e</sub>ω<sub>e</sub> = -5.441 × 10<sup>-3</sup>, z<sub>e</sub>ω<sub>e</sub> = -1.15 × 10<sup>-4</sup>, γ<sub>e</sub> = -1.535 × 10<sup>-5</sup>; (b) calculated by deperturbation analysis of A <sup>1</sup>Σ<sub>u</sub><sup>+</sup>; (c) y<sub>e</sub>ω<sub>e</sub> = -9.145 × 10<sup>-3</sup>, z<sub>e</sub>ω<sub>e</sub> = -5.02 × 10<sup>-5</sup>, γ<sub>e</sub> = -7.646 × 10<sup>-6</sup>

Dissociation energy = 0.75 ± 0.03 eV, 17.3 kcal/mole, 6049 cm<sup>-1</sup>.

Perturbations and General Information

Gyromagnetic ratio ( $g_J$ ) = 0.03892 nuclear magnetons (64.36).

A  $^1\Sigma_u^+$  state is perturbed by the b  $\Pi(0_u^+)$  state (33.21).

Radiative lifetimes:

$$A \ ^1\Sigma_u^+, \ \tau_r = 10^{-7} - 10^{-6} \text{ sec (70.44)}$$

$$B \ ^1\Pi_u, \ \tau_r = 6.41 \text{ nsec (69.43)}$$

Average polarizability (736°K) =  $30 \times 10^{-24} \text{ cm}^3$  (74.55).

Transition moment for  $B \ ^1\Pi_u \rightarrow X \ ^1\Sigma_g^+$  system (74.56):

$$D = 6.8 + 0.5r \quad 2.6\text{\AA} \leq r \leq 5.0\text{\AA}$$

Potential energy curves - RKR potential (69.40):

$T_e = 0.0$	State	v	$E(v) \text{cm}^{-1}$	$r_{\min}(\text{\AA})$	$r_{\max}(\text{\AA})$
	$X \ ^1\Sigma_g^+$	0	79.4	2.9481	3.2200
		1	237.2	2.8593	3.3320
		2	393.5	2.8014	3.4141
		3	548.?	2.7563	3.4841
		4	701.6	2.7187	3.5475
		5	853.4	2.6864	3.6065
		6	1003.6	2.6581	3.6624
		7	1152.3	2.6327	3.7163
		8	1299.3	2.6099	3.7686
		9	1444.9	2.5893	3.8196
		10	1588.8	2.5705	3.8699
		11	1731.0	2.5533	2.9195
		12	1871.7	2.5375	3.9687
		13	2010.7	2.5231	4.0176
		14	2148.0	2.5100	4.0665
		15	2283.6	2.4979	4.1153

State	v	E(v)cm <sup>-1</sup>	r <sub>min</sub> (A)	r <sub>max</sub> (A)
$T_e = 14680.4 \text{ cm}^{-1}$	A <sup>1</sup> $\Sigma_u^+$ 0	58.7	3.4875	3.8037
	1	175.5	3.3839	3.9330
	2	291.6	3.3159	4.0268
	3	406.9	3.2626	4.1060
	4	521.5	3.2179	4.1769
	5	635.3	3.1789	4.2421
	6	748.3	3.1442	4.3032
	7	860.6	3.1128	4.3612
	8	972.1	3.0839	4.4168
	9	1082.9	3.0573	4.4703
	10	1192.9	3.0324	4.5222
	11	1302.1	3.0091	4.5728
	12	1410.6	2.9871	4.6221
	13	1518.3	2.9663	4.6704
	14	1625.3	2.9466	4.7178
	15	1731.5	2.9278	4.7645
$T_e = 20319.596$	B <sup>1</sup> $\Pi_u$ 0	61.7	3.2663	3.5747
	1	184.2	3.1678	3.7044
	2	305.4	3.1038	3.7998
	3	425.1	3.0539	3.8814
	4	543.4	3.0122	3.9553
	5	660.2	2.9759	4.0242
	6	775.4	2.9435	4.0895
	7	889.0	2.9141	4.1523
	8	1000.9	2.8870	4.2132
	9	1111.1	2.8618	4.2727
	10	1219.5	2.8381	4.3313
	11	1326.0	2.8157	4.3892
	12	1430.6	2.7943	4.4467
	13	1533.2	2.7737	5.5039
	14	1633.9	2.7539	4.5612
	15	1732.4	2.7347	4.6186

Na<sub>2</sub>

Franck-Condon factors - RKR potential (69.41):

B<sup>1</sup>Π<sub>u</sub> - X<sup>1</sup>Σ<sup>+</sup><sub>g</sub>

v', v''	0	1	2	3	4	5	6	7	8
0	6.55-1	1.61-1	2.13-1	2.00-1	1.51-1	9.77-2	5.61-2	2.94-2	1.44-2
1	1.93-1	1.92-1	5.53-2	2.47-4	4.52-2	1.03-1	1.23-1	1.07-1	7.68-2
2	2.69-1	4.05-2	3.19-2	1.15-1	7.40-2	8.32-3	9.19-3	5.28-2	8.78-2
3	2.35-1	1.67-2	1.30-1	2.68-2	1.69-2	8.17-2	6.84-2	1.56-2	1.46-3
4	1.43-1	1.36-1	4.39-2	3.84-2	9.15-2	1.41-2	1.53-2	6.60-2	5.99-2
5	6.44-2	1.96-1	9.62-3	1.08-1	2.86-3	5.45-2	6.53-2	5.72-3	1.66-2
6	2.22-2	1.49-1	1.16-1	2.24-2	6.54-2	5.29-2	3.20-3	6.06-2	4.46-2
7	5.95-3	7.41-2	1.77-1	2.28-2	8.28-2	6.65-3	7.60-2	1.46-2	1.68-2
8	1.26-3	2.63-2	1.33-1	1.31-1	2.55-3	8.92-3	9.94-3	4.16-2	5.20-2

Franck-Condon factor followed by a factor of ten

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Nd<sub>2</sub>

Nd<sub>2</sub>

Spectroscopic Constants

Dissociation energy = 0.82 ± 0.30 eV, 19 kcal/mole, 6614 cm<sup>-1</sup> (72.1).

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Ne<sub>2</sub>Methods of Production and Experimental Technique

Absorption.

Discharge.

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_0, 0$	Remarks	Bibliography
	I	A( $\text{C}_u^+$ ) - X <sup>1</sup> $\Sigma_g^+$ ( $0_g^+$ )	Absorption	747-745	V			(72.5)
	II	B( $0_u^+$ ) - X <sup>1</sup> $\Sigma_g^+$	Absorption	737-736	V			(72.5)
	III	C( $1_u$ ) - X <sup>1</sup> $\Sigma_g^+$	Absorption	639-630				(72.5)
	IV	D( $0_u^+$ ) - X <sup>1</sup> $\Sigma_g^+$	Absorption	631-629				(72.5)
	V	E( $0_u^+$ ) - X <sup>1</sup> $\Sigma_g^+$	Absorption	628-626				(72.5)
	VI	F( $0_u^-$ )? - X <sup>1</sup> $\Sigma_g^+$	Absorption	629-627				(72.5)
	VII	G( $0_u^+$ ) - X <sup>1</sup> $\Sigma_g^+$	Absorption	624-619				(72.5)
	VIII	H( $0_u^+$ ) - X <sup>1</sup> $\Sigma_g^+$	Absorption	624-619				(72.5)
	IX	I( $0_u^+$ )? - X <sup>1</sup> $\Sigma_g^+$	Absorption	618-615				(72.5)
	X	J( $1_u$ ) - X <sup>1</sup> $\Sigma_g^+$	Absorption	609-603				(72.5)
	XI	K( $0_u^+$ ) - X <sup>1</sup> $\Sigma_g^+$	Absorption	604-602				(72.5)

Molecule Ne<sub>2</sub>

**Ne<sub>2</sub>****BAND SYSTEMS**

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
	XII	L( $0_u^+, 0_u^-$ ) -	Absorption	601-600				(72.5)

Molecule Ne<sub>2</sub>

I. A(0<sub>u</sub><sup>+</sup>) ← X<sup>1Σ<sup>+</sup> g(0<sub>g</sub><sup>+</sup>) System</sup>

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)	(v-3, 0)
λ	745. 11	745. 34	745. 85	746. 83
(Intensity)	10	3	4	0

II. B(0<sub>u</sub><sup>+</sup>) ← X<sup>1Σ<sup>+</sup> g System</sup>

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v, 1)	(v-1, 0)	(v-1, 1)
λ	736. 18	736. 25	736. 49	736. 57
(Intensity)	10	8	3	1

III. C(1<sub>u</sub>) ← X<sup>1Σ<sup>+</sup> g System</sup>

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)	(v-3, 0)	(v-4, 0)	(v-5, 0)
λ	630. 98	631. 49	632. 05	632. 71	633. 45	634. 26
(Intensity)	10	9	8	6	4	2

VI. D(0<sub>u</sub><sup>+</sup>) ← X<sup>1Σ<sup>+</sup> g System</sup>

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)
λ	629. 87	630. 06	630. 27
(Intensity)	4	6	10

V. E(0<sub>u</sub><sup>+</sup>) ← X<sup>1Σ<sup>+</sup> g System</sup>

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)	(v-3, 0)
λ	626. 92	627. 03	627. 23	627. 46
(Intensity)	2	5	6	10

$\text{Ne}_2$

VI.  $F(0_u^-) \leftarrow X^1\Sigma_g^+ \text{ System}$

Band heads,  $\lambda$  (Intensity) (72.5):

$(v', v'')$	$(v, 0)$	$(v-1, 0)$	$(v-2, 0)$	$(v-2, 1)$	$(v-3, 0)$
$\lambda$	619.26	619.62	620.07	620.13	620.61
(Intensity)	10	7	6	2	5

VII.  $G(0_u^+) \leftarrow X^1\Sigma_g^+ \text{ System}$

Band heads,  $\lambda$  (Intensity) (72.5):

$(v', v'')$	$(v, 0)$	$(v-1, 0)$	$(v-2, 0)$	$(v-3, 0)$
$\lambda$	619.42	619.80	620.28	620.82
(Intensity)	10	7	4	2

VIII.  $H(0_u^+) \leftarrow X^1\Sigma_g^+ \text{ System}$

Band heads,  $\lambda$  (Intensity) (72.5):

$(v', v'')$	$(v, 0)$	$(v-1, 0)$	$(v-2, 0)$	$(v-3, 0)$
$\lambda$	619.42	619.80	620.28	620.82
(Intensity)	10	7	4	2

IX.  $I(0_u^+) \leftarrow X^1\Sigma_g^+ \text{ System}$

Band heads,  $\lambda$  (Intensity) (72.5):

$(v', v'')$	$(v, 0)$	$(v-1, 0)$	$(v-2, 0)$	$(v-3, 0)$
$\lambda$	616.30	616.53	616.81	617.06
(Intensity)	10	5	8	3

X.  $J(1_u) \leftarrow X^1\Sigma_g^+ \text{ System}$

Band heads,  $\lambda$  (Intensity) (72.5):

$(v', v'')$	$(v-1, 0)$	$(v-2, 0)$	$(v-3, 0)$	$(v-4, 0)$
$\lambda$	603.57	603.85	604.28	604.74
(Intensity)	10	8	7	7

XI. K(0<sup>+</sup><sub>u</sub>) - X<sup>1Σ<sup>+</sup><sub>g</sub> System</sup>

Band heads, λ (Intensity) (72.5):

(v', v'')	(v, 0)	(v-1, 0)	(v-2, 0)	(v-3, 0)	(v-4, 0)
λ	602.88	602.90	602.97	603.08	603.23
(Intensity)	6	4	5	6	10

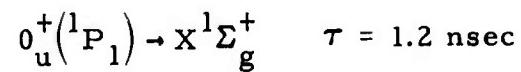
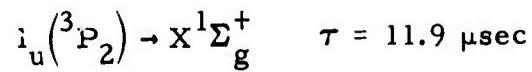
## SPECTROSCOPIC CONSTANTS

State	T <sub>e</sub>	$\omega_e$	$x_e \omega_e$	B <sub>e</sub>	$\alpha_e \times 10^3$	D <sub>e</sub> × 10 <sup>6</sup>	r <sub>e</sub>	Remarks	Bibliography
X <sup>1Σ<sup>+</sup></sup>	0	31.3	6.84	0.20	60		2.91		(72.5)

Dissociation energy =  $3.74 \times 10^{-3}$  eV, 10.6 cal/mole,  $30.2 \text{ cm}^{-1}$  (72.5).

Perturbations and General Information

Radiative lifetimes - calculated (74.15):



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Ni<sub>2</sub>

Ni<sub>2</sub>

Spectroscopic Constants

Dissociation energy = 2.37 ± 0.22 eV, 54.5 kcal/mole, 19100 cm<sup>-1</sup> (64.1).

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O<sub>2</sub>

O<sub>2</sub>

### Methods of Production and Experimental Technique

Absorption: in high frequency discharges, pulsed discharges, ac discharges, flash photolysis.

Emission: all types of discharges, flames, explosions, luminescence.

In astrophysics.

Ground state studied by microwave spectroscopy.

### BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, v, 0	Remarks	Bibliography
Infrared atmospheric	I	a <sup>1</sup> Δ <sub>g</sub> ≈ X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	Absorption, emission	15800-9240	R	7882. 39		(72.73, 62.39, 59.32, 58.29, 47.14, 33.6)
	II	b <sup>1</sup> Σ <sub>g</sub> <sup>+</sup> ≈ X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	Absorption, emission	9970-5380	R	13120. 9085		(72.73, 69.57, 64.41, 61.36, 50.18, 49.17)
	III	b <sup>1</sup> Σ <sub>g</sub> <sup>+</sup> → a <sup>1</sup> Δ <sub>g</sub>	Discharge	19080		5240 (head)	Only a single band	(69.57)
	IV	c <sup>1</sup> Σ <sub>u</sub> <sup>-</sup> ≈ X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	Absorption, lumines- cence	4790-4490 2715-2540	R	32664. 1 (calculated)		(68.49, 53.22)
	V	C <sup>3</sup> Δ <sub>u</sub> ≈ X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	Absorption at high pressure	2630-2570 2924-2440	R	34319 (head)		(53.22, 39.11, 34.8, 32.5, 28.1)

Molecule O<sub>2</sub>

O<sub>2</sub>

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $v_{0,0}$	Remarks	Bibliography
Chamberlain Herzberg I Schumann- Runge	VI	C <sup>3</sup> Δ <sub>u</sub> - a <sup>1</sup> Δ <sub>g</sub>	Lumines- cence	4380-3700	R			(58.27)
	VII	A <sup>3</sup> Σ <sub>u</sub> <sup>+</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	Absorption, lumines- cence	4880-2430	R	35007.15 (calculated)		(60.33, 59.31, 57.26, 55.25)
	VIII	B <sup>3</sup> Σ <sub>u</sub> <sup>-</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	All sources	5350-1750 1750-1300	R Continuum	49358.15		(72.73, 68.54, 68.52, 66.45, 64.43, 64.42, 61.35, 59.30, 54.24, 54.23, 50.19)
	IX	a <sup>1</sup> Σ <sub>u</sub> <sup>+</sup> - b <sup>1</sup> Σ <sub>g</sub> <sup>+</sup>		1585-1538	V	63141.5		(68.48)
		a <sup>1</sup> Σ <sub>u</sub> <sup>+</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>		1280-1196	V			(69.58, 68.48)
		b <sup>3</sup> Σ <sub>u</sub> <sup>+</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	Absorption	1294-1181	V			(69.58, 68.48, 52.21)
		1Δ <sub>u</sub> - a <sup>1</sup> Δ <sub>g</sub>		1243.8 (only a single band)		80396.0		(68.48)

Molecule O<sub>2</sub>

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $v_{0,0}$	Remarks	Bibliography
Rydberg Series	IX (cont)	1Π <sub>u</sub> - a <sup>1</sup> Δ <sub>g</sub>		1229.0 (only a single band)		81362.5		(68.48)
		3Σ <sub>u</sub> <sup>+</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>		1144.6 (only a single band)	V	87369.1		(69.58)
	X	X <sup>2</sup> Π <sub>g</sub> <sup>(0+)</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>		1290-1180	V			(61.38, 52.21)
		b <sup>4</sup> Σ <sub>g</sub> <sup>-</sup> <sup>(0+)</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	Absorption	730-660	R			(68.51, 33.9)
		B <sup>2</sup> Σ <sub>g</sub> <sup>-</sup> <sup>(0+)</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>		650-600	R			(68.51, 68.50, 42.12)
		c <sup>4</sup> Σ <sub>u</sub> <sup>-</sup> <sup>(0+)</sup> - X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>		595-510				(69.61)
	XI	Many bands that are unclassified or whose identification is doubtful						(68.51, 68.48, 67.47, 61.37, 54.24, 52.21, 48.16, 43.13)

Molecule O<sub>2</sub>

I.  $a^1\Delta_g \rightleftharpoons X^3\Sigma_g^-$  System (Infrared Atmospheric)

Band origins,  $\lambda$  (58.29, 47.14, 33.6):

$(v', v'')$	$(0, 1)$	$(0, 0)$	$(1, 0)$	$(2, 0)$
$\lambda$	(15800)	1263.0	10674.1	(9240)

II.  $b^1\Sigma_g^+ \rightleftharpoons X^3\Sigma_g^-$  System (Atmospheric)

Band heads in emission,  $\lambda$  (69.57, 64.41, 61.36, 50.18, 49.17):

$v', v''$	0	1	2	3	4
0	7593.73	(8623)	(9970)		
1	6867.2	7683.85	8697.8		
2	6276.6	6953	7779.03		
3			7043	7879.17	
4				7141	7987

III.  $b^1\Sigma_g^+ \rightarrow a^1\Delta_g$  System (Noxon)

Only a single band, Q branch (69.57):

$$\lambda(0, 0) | 19080$$

IV.  $c^1\Sigma_u^- \rightleftharpoons X^3\Sigma_g^-$  System (Herzberg II)

Band origins (calculated),  $\lambda$  (68.49):

$v', v''$	0	1	2	3	4	5	6	7	8
0	3060.6	3213.7	3380.3	3562.0	3761.2	3980.3	4222.4	4491.2	(a) 4791.5 (a)
1	2990.3	3136.3	3294.7	3467.2	3655.6	3862.2	4089.7	4341.5	4621.4
2	2925.5	3065.1	3216.2	3380.4	3559.2	3754.8	3969.5	4206.2	4468.5
3	2865.8	2999.7	3144.3	3301.0	3471.3	3657.1	3860.5	4084.0	4330.8
4	2811.0	2939.6	3078.4	3228.4	3391.1	3568.2	3761.6	3973.5	4206.7
5	2760.6	2884.6	3018.1	3162.1	3318.1	3487.5	3671.9	3873.6	4094.9
6	2714.5 <sup>(b)</sup>	2834.2	2963.0	3101.8	3251.7	3414.2	3590.8	3783.4	3994.2
7	2672.3 <sup>(b)</sup>	2788.3	2912.9	3046.9	3191.4	3347.8	3517.4	3702.0	3903.6
8	2634.0 <sup>(b)</sup>	2746.6	2867.4	2997.1	3136.9	3287.8	3451.3	3628.8	3822.4
9	2599.2 <sup>(b)</sup>	2708.9	2826.2	2952.2	3087.7	3233.9	3391.9	3563.2	3749.6
10	2568.0 <sup>(b)</sup>	2674.9	2789.3	2911.9	3043.7	3185.6	3338.8	3504.7	3684.9

(a) Observed in luminescence, (b) observed in absorption (53.22)

O<sub>2</sub>

V. C<sup>3</sup>Δ<sub>u</sub> ← X<sup>3</sup>Σ<sup>-</sup><sub>g</sub> System (Herzberg III, High Pressure Bands)

Herzberg III

Two fragments with three heads have been observed (53.24).  
Vibrational numbering is uncertain.

(v', v'')	F <sub>2</sub> (6, 0)	F <sub>3</sub> (6, 0)	(5, 0)
λ	2589. 14	2579. 39	2620. 71

High Pressure Bands (diffuse)

Maxima in absorption (no heads), λ (39.11).  
Vibrational numbering is uncertain.

(v', v'')	(0,0)	(1,0)	(2,0)	(3,0)	(4,0)	(5,0)	(6,0)	(7,0)	(8,0)	(9,0)
λ	2924	2855	2795	2739.8	2689.8	2642.7	2598.8	2555.9	2525.4	2497.4
	2913	2842	2783.9	2729.9	2679.3	2632.7	2590.3	2553.5	2517	2488.7
	2904	2832	2769.1	2720.7	2671.6	2626	2582.4	2537	2510	2482

VI. C<sup>3</sup>Δ<sub>u</sub> → a<sup>1</sup>Δ<sub>g</sub> System (Chamberlain)

27 weak bands have been observed, but the identification is uncertain.  
Vibrational numbering of the lower state is uncertain.

Possible band heads, λ (53.24):

v', v''	0	1	2	3	4	5
0						
1			4135			
2						
3			3887	4114		
4					4244	
5			3698		4127	4378
6				3813	4031	

O<sub>2</sub>

v', v''	0	1	2	3	4	5
0						
1			4107			
2						
3			3866	4090		
4					4221	
5					4107	
6				3792	4009	4240

v', v''	0	1	2	3	4	5
0						
1			4086			
2						
3			3844	4071	4317	
4						
5				3861	4086	4326
6				3771	3985	4215

O<sub>2</sub>

VII. A<sup>3Σ<sup>+</sup></sup> ≈ X<sup>3Σ<sup>-</sup> System (Herzberg I)</sup>

Band heads in emission, λ (Intensity) (59.31):

v', v''	0	1	2	3	4	5	6	7	8
0						3840 (5)	4064 (5)	4309 (7)	
1				(3366.5) (2)	3542 (8)	3734 (8)	3938 (7)	4170 (6)	
2				3285 (7)	3453 (8)	3633 (8)	3829 (8)	4044 (2)	
3	2931 (1)	3066 (5)	3211 (10)		3370 (10)	3542 (8)	(3726.1) (2)	(3842.2) (2)	
4	2873 (2)	3002 (5)	3142 (7)		3292 (4)	3459 (2)	(3634.6) (2)		
5	2820 (3)	2945 (5)	3080 (2)		(3225.0) (2)		(3552.5) (4)	(3737.7) (4)	
6	2775 (3)	2895 (6)	3026 (2)			(3315.7) (2)	(3479.3) (4)	3657 (2)	
7	2622 (3)	2734 (5)	2850 (5)			(3257.1) (4)	(3414.7) (4)		
8	2588 (2)	2696 (4)							

VIII. B<sup>3Σ<sup>-</sup></sup> ≈ X<sup>3Σ<sup>-</sup> System (Schumann-Runge)</sup>

Band origins in absorption, λ (68.54, 66.45, 64.43, 64.42, 59.30, 54.23, 50.19):

v', v''	0	1	2	3	4	5	6	7	8
0	2026.01								
1	1998.17							2522.67	2614.67
2	1971.97	2034.29				2316.82	2396.80	2481.02	2569.95
3	1947.33	2008.11				2282.89	2360.52	2442.25	
4	1924.19	1983.60		2110.91	2179.36	2251.21	2326.53		
5	1902.23	1960.58	2021.28	2084.93	2151.61	2221.53	2295.03		
6	1882.43	1939.25	1998.63	2060.84	2125.94	2194.20			
7	1863.72	1919.37	1977.57	2038.35	2102.05	2168.78			
8	1846.51	1901.14	1958.21	2017.84	2080.22	2145.54			
9	1830.76	1884.47	1940.47	1999.05	2060.27	2124.31			
10	1816.50	1869.37	1924.48	1982.02	2042.23	2105.05			

IX. Partial Systems $\alpha^1\Sigma_u^+ \leftarrow b^1\Sigma_g^+$  SystemBand heads,  $\lambda$  (68.48):

$$(v', v'') \quad (0, 0) \quad (1, 1) \quad (1, 0)$$

$$\lambda \quad 1583.9 \quad 1571.9 \quad 1537.9$$

 $\alpha^1\Sigma_u^+ \leftarrow X^3\Sigma_g^-$  SystemBand heads,  $\lambda$  (69.58, 68.48):

$$(v', v'') \quad (1, 0) \quad (2, 0) \quad (3, 0) \quad (4, 0)$$

$$\lambda \quad 1279.5 \quad 1250.0 \quad 1222.1 \quad 1196.4$$

 $\beta^3\Sigma_u^+ \leftarrow X^3\Sigma_g^-$  SystemBand origins,  $\lambda$  (69.58, 68.48):

$$(v', v'') \quad (2, 0) \quad (3, 0)$$

$$\lambda \quad 1262.18 \quad 1233.47$$

 $^1\Delta_u \leftarrow a^1\Delta_g$  SystemBand head,  $\lambda$  (68.48):

$$(v', v'') \quad (0, 0)$$

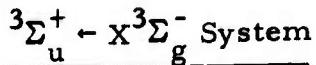
$$\lambda \quad 1243.8$$

 $^1\Pi_u \leftarrow a^1\Delta_g$  SystemBand head,  $\lambda$  (68.48):

$$(v', v'') \quad (0, 0)$$

$$\lambda \quad 1229.0$$

O<sub>2</sub>

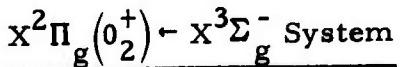


Double headed bands with 3 branches. Band head,  $\lambda$  (69.58):

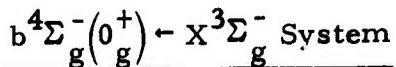
$$\begin{array}{ll} (v', v'') & (0, 0) \\ \lambda & 1144.6 \end{array}$$

X.

Rydberg Series



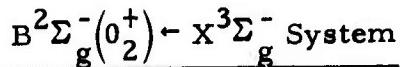
Single progression of doublets. Classification is doubtful (61.38, 52.21).



Many progressions with the proposed configuration  $\cdots np \sigma_u^- ^3\Sigma_u^-$  have been observed (68.38, 62.40, 35.9).

$$\text{Band head formula: } v = 146568 - \frac{R}{(n-1.679)^2} \quad (n = 5 \cdots \infty)$$

Another weak, diffuse series has been observed with a proposed configuration of  $np \pi_u^- ^3\Pi_u^-$  (68.38).



Bands with simple heads (68.51, 68.50, 42.12).

$$\text{Band head formula: } v = 163602 - \frac{R}{(n-0.658)^2} \quad (n = 4 \cdots \infty)$$

c  $^4\Sigma^-$  (0<sup>+</sup>)  $\leftarrow$  X  $^3\Sigma^-$  g System

Several series have been observed (69.61).

$\Pi$  Series - probably excited to the nd  $\pi_g$   $^3\Pi_u$  Rydberg state.

$$\text{Band head formula: } v = 198125 - \frac{R}{(n-1.559)^2} \quad (n = 4 \dots \infty)$$

$\Sigma$  Series - probably excited to the ns  $\sigma_g$   $^3\Sigma_u^-$  Rydberg state.

$$\text{Band head formula: } v = 198125 - \frac{R}{(n-0.955)^2} \quad (n = 4 \dots \infty)$$

SPECTROSCOPIC CONSTANTS

Molecule

$\text{O}_2$

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^2$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$1\Pi_u$	89244.9 (a)			(1.451)					(68.48)
$1\Delta_u$	88278.4 (a)			(1.446)					(68.48)
$3\Sigma_u^+$	87369.1 (a)			(1.706)					(69.58)
$\alpha^1\Sigma_u^+$	76089	(1927)	(19)	1.599	1.6				(69.58, 68.48)
$\beta^3\Sigma_u^+$	75263	(1957)	(19.7)	(1.7)	(2)				(69.58, 68.48, 52.21)
$B^3\Sigma_u^-$	49794.33	709.058	10.6141	0.818975	1.19225				(70.63, 66.45, 54.23, 34.7)
$A^2\Sigma_u^+$	35398.70	799.08	12.16	0.91053	1.416	4.79	1.52153	(c, h)	(54.24, 52.20)
$C^3\Delta_{u,i}$	34735	(750)	(14)						(53.22, 39.11, 32.5)
$c^1\Sigma_u^-$	33058.4	794.29	12.736	0.9155	1.391	(10.5)	1.5174	(d, i)	(68.49, 53.22)
$b^1\Sigma_g^+$	13195.314	1432.66	13.9336	1.4004796	1.8169303	5.356	1.22684	(e, j)	(n.p. 175, 48.15)
$a^1\Delta_g$	7918.11	(1509.3)	12.9	1.4263	1.71	(4.97)	1.21567		(47.14)

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## SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^2$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$X^3\Sigma^-_g$	0	1580.19	11.981	1.445622	1.593268	1.20754	(f, k)	(n.p. 125, 66.45, 54.23, 34.7)	

(a)  $T_e$ ; (b)  $y_e \omega_e = -0.059212435$ ,  $z_e \omega_e = -0.023974994$ ; (c)  $y_e \omega_e = -0.550$ ; (d)  $y_e \omega_e = -0.2444$ ,  $z_e \omega_e = 0.00055$ ;

(e)  $y_e \omega_e = -0.0143$ ; (f)  $y_e \omega_e = 0.047474736$ ,  $z_e \omega_e = -0.00012727481$ ; (g)  $\gamma_e = -6.30472 \times 10^{-4}$ ;

(h)  $\gamma_e = -9.7 \times 10^{-4}$ ,  $\beta_e = 3.0 \times 10^{-7}$ ; (i)  $\gamma_e = -7.40 \times 10^{-4}$ ; (j)  $\gamma_e = -4.2941920 \times 10^{-5}$ ,  $\beta_e = 0.077$ ;

(k)  $\gamma_e = 6.406456 \times 10^{-5}$

Dissociation energy =  $5.12 \pm 0.0019$  eV, 117.97 kcal/mole,  $41260 \text{ cm}^{-1}$  (54.23).

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## Perturbations and General Information

Ionization potential ( $I_p$ ) to  $X^2\Pi_{g,i}(0_2^+)$  =  $12.059 \pm 0.001$  eV (68.53, 66.44).

$A^3\Sigma_u^+ - X^3\Sigma_g^-$  has a strong perturbation in the (11,0) band for  $N > 11$  (52.20).

$B^3\Sigma_u^-$  state is perturbed at  $v = 16$ ,  $J = 8$  and  $v = 19$ ,  $J = 8$  (54.23).

$B^3\Sigma_u^-$  state is predissociated, probably by a repulsive  $^3\Pi_u$  state. The predissociation is characterized by an onset at  $v = 2$  and broadening at  $v = 4, 8$ , and 11, with a minimum at  $v = 9$ . The interpretation of the predissociation is in question (72.73, 70.62, 69.60, 69.59, 61.36, 59.30, 58.28, 36.10).

Vibrational Raman effect has been observed (60.33, 30.3, 29.2).

Rotational Raman effect has been observed (74.114, 60.33, 30.3).

Potential energy curves – RKR potentials (72.73 and references cited therein):

State	v	V(cm <sup>-1</sup> )	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)
$X^3\Sigma_g^-$ $T_e = 0 \text{ cm}^{-1}$	0	787.3818	1.1590417	1.2626908
	1	2343.7613	1.1272513	1.3078976
	2	3876.57	1.10700	1.34170
	3	5386.03	1.09146	1.37093
	4	6872.34	1.07864	1.39759
	5	8335.65	1.06767	1.42257
	6	9776.11	1.0580	1.4464
	7	11193.80	1.0494	1.4693
	8	12588.82	1.0417	1.4917
	9	13961.18	1.0346	1.5136
$a^1\Delta_g$ $T_e = 7918.11 \text{ cm}^{-1}$	10	15310.91	1.0280	1.5351
	0	751.658	1.16619	1.27228
	1	2235.158	1.13396	1.31904
	2	3692.86	1.11353	1.35422
$b^1\Sigma_g^+$ $T_e = 13195.314 \text{ cm}^{-1}$	3	5124.76	1.0979	1.3848
	0	712.9766	1.176241	1.285186
	1	2117.7290	1.143442	1.333696
	2	3494.4855	1.122734	1.370428
	3	4843.1603	1.106952	1.402561

State	v	V(cm <sup>-1</sup> )	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)
$A^3\Sigma_u^+$	0	395.8	1.454	1.600
	1	1168.7	1.411	1.668
	2	1912.5	1.385	1.722
	3	2623.5	1.366	1.772
	4	3298.9	1.350	1.822
	5	3934.9	1.337	1.872
	6	4527.2	1.326	1.925
	7	5070.0	1.317	1.982
	8	5555.6	1.310	2.050
	9	5973.4	1.304	2.131
	10	6309.1	1.298	2.245
$B^3\Sigma_u^-$	0	351.204	1.53266	1.68771
	1	1038.736	1.48649	1.75876
	2	1703.961	1.45776	1.81426
	3	2345.774	1.43623	1.86450
	4	2962.845	1.41889	1.91257
	5	3553.643	1.40434	1.96005
	6	4118.425	1.39181	2.00806
	7	4649.207	1.38084	2.05761
	8	5149.746	1.37117	2.10976
	9	5615.548	1.36264	2.16578
	10	6043.932	1.35518	2.22722
	11	6432.167	1.34876	2.29602

Radiative lifetimes, Einstein coefficients and oscillator strengths:

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Transition	Band	$\tau$ (sec)	$A_{\nu'} (\text{sec}^{-1})$	$A_{\nu' \nu''} (\text{sec}^{-1})$	Absorption $f$ -value	Reference
a $^1\Delta_g - X^3\Sigma_g^-$	0 - 0	$3.88(10^3)$	$2.58(10^{-4})$	$4.15(10^{-12})$	(68.55)	
b $^1\Sigma_g^+ - X^3\Sigma_g^-$	0 - 0		0.085	$2.47(10^{-10})$	(67.46)	
	1 - 0			(0.0069)	(32.4)	
	2 - 0			$(0.1636) 10^{-3}$	(68.56)	
	1 - 1		0.0704		(68.56)	
c $^1\Sigma_g^+ - a^1\Delta_g$	0 - 0			$1.5(10^{-3})$	(61.34)	
A $^3\Sigma_u^+ - X^3\Sigma_g^-$			$(1 - 10^3)$		(67.46, 64.41, 62.40)	
	7 - 0			$1.24(10^{-10})$	(70.64)	
c $^1\Sigma_u^- - X^3\Sigma_g^-$			$\sim 10^{-4}$		(62.40)	
			$> 10^{-3}$		(64.41)	
C $^3\Delta_u - X^3\Sigma_g^-$				$\leq 10^{-5}$	(62.40)	
				$> 10^{-3}$	(64.41)	

Absolute *f*-values for the B<sup>3Σ<sub>u</sub><sup>-</sup> - X<sup>3Σ<sub>g</sub><sup>-</sup> bands (72.73 and references cited therein):</sup></sup>

v', v''	0	1	2
0	3. 45-10		
1	3. 90-9		
2	2. 38-8	5. 35-7	
3	9. 90-8	2. 08-6	
4	3. 21-7	6. 15-6	
5	8. 52-7	1. 53-5	
6	1. 91-6	3. 15-5	2. 13-4
7	3. 81-6	5. 78-5	3. 39-4
8	6. 68-6	9. 40-5	5. 46-4
9	1. 06-5	1. 38-4	9. 87-4
10	1. 57-5	1. 91-4	1. 03-3
11	2. 09-5	2. 38-4	1. 04-3
12	2. 53-5	2. 73-4	1. 22-3
13	2. 88-5	2. 93-4	1. 04-3
14	3. 03-5	2. 95-4	
15	2. 92-5	2. 77-4	
16	2. 59-5	2. 42-4	
17	2. 23-5	2. 01-4	
18	1. 83-5		
19	1. 44-5		

*f*-value followed by a factor of ten

Franck-Condon factors - RKR potentials (n.p. 125, 72.73):

a<sup>1Δ<sub>g</sub></sup> - X<sup>3Σ<sub>g</sub><sup>-</sup></sup>

v', v''	0	1	2	3	4
0	9. 869-1	1. 297-2	1. 260-4		
1	1. 303-2	9. 586-1	2. 791-2	4. 296-4	1. 735-6
2	6. 795-5	2. 814-2	9. 258-1	4. 497-2	9. 802-4
3	2. 591-4	4. 548-2	8. 881-1	6. 423-2	1. 867-3

Franck-Condon factors followed by a factor of ten

$O_2$ 
 $b^1\Sigma^+ - X^3\Sigma^-$   
 $g$        $g$ 

$v', v''$	0	1	2	3	4	5	6
0	9. 308-1	6. 660-2	2. 523-3	5. 648-5			
1	6. 647-2	7. 928-1	1. 322-1	8. 284-3	2. 736-4	6. 417-6	
2	2. 639-3	1. 315-1	6. 527-1	1. 943-1	1. 802-2	8. 232-4	2. 512-5
3	6. 911-5	8. 753-3	1. 924-1	5. 144-1	2. 499-1	3. 240-2	1. 968-3

Franck-Condon factors followed by a factor of ten

 $A^3\Sigma^+ - X^3\Sigma^-$   
 $u$        $g$ 

$v', v''$	6	7	8	9	10	11	12
0	4. 260-2	7. 935-2	1. 214-1	1. 546-1	1. 654-1	1. 495-1	1. 140-1
1	8. 985-2	1. 052-1	8. 298-2	3. 500-2	1. 510-3	1. 512-2	6. 765-2
2	8. 158-2	4. 457-2	4. 492-3	1. 049-2	5. 486-2	7. 589-2	4. 343-2
3	3. 593-2	1. 434-3	1. 700-2	5. 478-2	4. 681-2	6. 822-3	9. 761-3
4	3. 900-3	1. 162-2	4. 595-2	3. 559-2	1. 700-3	1. 847-2	5. 157-2

Franck-Condon factors followed by a factor of ten

 $B^3\Sigma^- - X^3\Sigma^-$   
 $u$        $g$ 

$v', v''$	12	13	14	15	16	17
0	1. 192-1	1. 443-1	1. 514-1	1. 378-1	1. 087-1	7. 417-2
1	6. 350-2	2. 328-2	3. 441-4	1. 553-2	6. 165-2	1. 087-1
2	5. 507-5	1. 853-2	5. 696-2	6. 930-2	3. 928-2	3. 934-3
3	3. 150-2	5. 446-2	3. 492-2	2. 823-3	1. 221-2	5. 283-2
4	4. 503-2	1. 900-2	1. 904-4	2. 620-2	4. 910-2	2. 392-2
5	1. 579-2	6. 553-4	2. 667-2	3. 844-2	9. 388-3	5. 262-3

Franck-Condon factors followed by a factor of ten

 $b^1\Sigma^+ - a^1\Delta_g$   
 $g$ 

$v', v''$	0	1	2	3
0	9. 770-1	2. 283-2	2. 136-4	
1	2. 267-2	9. 290-1	4. 760-2	7. 217-4
2	3. 628-4	4. 694-2	8. 768-1	7. 430-2
3	4. 426-6	1. 213-3	7. 266-2	8. 202-1

Franck-Condon factors followed by a factor of ten

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Methods of Production and Experimental Technique

Absorption in phosphorus vapor, flash photolysis of PH<sub>3</sub>.

Emission from a discharge of He or H<sub>2</sub> with phosphorus, discharge in PH<sub>3</sub> or microwave discharge in PCl<sub>3</sub>.

Fluorescence.

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
	I	A <sup>1</sup> $\Pi_g \rightarrow X^1\Sigma_g^+$	Emission	3110-2850	R	2970(0, 1)		(73.42, 58.21)
	II	C <sup>1</sup> $\Sigma_u^+ \approx X^1\Sigma_g^+$	Emission	3500-2000	R	2953.6(6, 22) 2757.1(4, 17) 2456.9(3, 10) 2108.1(3, 1)		(67.31, 67.30, 66.24, 64.23, 61.22, 50.18, 50.17, 49.16, 46.14, 43.12, 43.11, 40.10, 35.9, 33.8, 32.7, 32.6, 32.5, 32.4, 31.3, 30.2, 07.1)
			Absorption	2300-1800	R			
	III	E <sup>1</sup> $\Pi_u \approx X^1\Sigma_g^+$	Absorption, emission	1750-1600	R	1705.5(0, 1) 1728.1(0, 2)		(66.24, 55.20, 55.19)
	IV	G <sup>1</sup> $\Sigma_u^+ \approx X^1\Sigma_g^+$	Absorption, emission	1530-1480	R	1508.7(0, 0)		(66.24, 55.19)
	V	I <sup>1</sup> $\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	1480-1460	R	1460.7(0, 0)		(66.24)
	VI	K <sup>1</sup> $\Pi_u \leftarrow X^1\Sigma_g^+$	Absorption	1400-1320	R	1384.0(0, 0)		(66.24)
	VII	M <sup>1</sup> $\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Absorption	1350-1300	R	1355.1(0, 0)		(66.24)
	VIII	N <sup>1</sup> $\Sigma_u^+ \leftarrow X^1\Sigma_g^+$	Absorption	1310-1290	R	1294.5(0, 0)		(66.24)

Molecule P<sub>2</sub>

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
	IX	$Q^1\Pi_u \rightarrow X^1\Sigma_g^+$	Absorption	~ 1250	R	1253.5(0, 0)		(66.24)
	X	$S^1\Sigma_g^+ \rightarrow X^1\Sigma_g^+$	Absorption	~ 1227	R	1227.6		(66.24)
	XI	$b^3\Sigma_u^- \rightarrow X^1\Sigma_g^+$	Emission	4400-3500	R	3720.1(0, 2) 3828.8(0, 3)		(74.44, 67.29)
	XII	$B^1\Pi_u \rightarrow A^1\Pi_g$	Emission	6674-6270		6414.0(0, 0)		(72.42, 71.40)
	XIII	$c(^3\Pi_u) \rightarrow b(^3\Pi_g)$	Emission	10050-7700	V	8622.0(4, 2) 8738.9(4, 2) 8829.2(4, 2)		(68.32, 67.29, 67.27, 64.23)

Molecule P<sub>2</sub>

I.  $A^1\Pi_g \rightarrow X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (58.21):

$(v', v'')$	$(0, 3)$	$(0, 2)$	$(0, 1)$	$(0, 0)$	$(1, 0)$
$\lambda$	3112.45	3039.29	2969.84	2902.99	2852.23

II.  $C^1\Sigma_u^+ \approx X^1\Sigma_g^+$  System

Band heads,  $\lambda$

$v', v''$	0	1	2	3	4	5	6	7
0	2136.58				2286.36	2326.5	2367.6	2409.9
1	2115.23	2150.0	2186.4		2261.6	2301.0		
2	2094.38	2128.6		2164.3			2315.97	2356.3
3	2074.66	2108.1			2143.0	2253.24	2291.8	
4	2055.32	2088.3		2157.35		2122.6	2267.86	
5	2036.55	2069.0			2172.2		2245.4	2283.2
6	2018.08	2050.0					2223.0	
7	2000.26					2165.9		
8	1983.52					2145.31	2180.43	2216.1
9	1966.61		2027.52		2092.21		2159.89	2195.01
10	1950.15		2009.80			2073.56		

III.  $E^1\Pi_u \approx X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (66.24, 55.19):

$v', v''$	0	1	2	3	4
0	1683.22	1705.47	1728.14	1751.23	
1	1663.76		1709.6	1732.24	1755.10
2	1644.92				
3	1626.65				
4	1608.89				

IV.  $G^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (66.24, 55.19):

$v', v''$	0	1	2	3	4	5
0	1508.68	1526.50				
1	1493.30	1510.75	1528.45			
2	1478.39	1495.51	1512.85	1530.54		
3		1480.74	1497.77	1515.07		
4				1500.12	1517.33	
5					1502.53	1519.67
6						

V.  $I^1\Pi_u^- \leftarrow X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (66.24):

$$\begin{array}{ccc} (v', v'') & (0, 1) & (0, 0) \\ \lambda & 1477.42 & 1460.69 \end{array}$$

VI.  $K^1\Pi_u^- \leftarrow X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (66.24):

$$\begin{array}{ccccccc} (v', v'') & (0, 1) & (0, 0) & (1, 0) & (2, 0) & (3, 0) & (4, 0) \\ \lambda & 1398.98 & 1383.98 & 1370.67 & 1357.81 & 1345.17 & 1333.16 \end{array}$$

VII.  $M^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (66.24):

$$\begin{array}{ccccccc} (v', v'') & (0, 0) & (1, 0) & (2, 0) & (3, 0) & (4, 0) \\ \lambda & 1355.06 & 1342.82 & 1330.92 & 1319.33 & 1308.04 & \end{array}$$

VIII.  $N^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (66.24):

$$\begin{array}{cccccccc} (v, v'') & (1, 2) & (0, 1) & (2, 2) & (1, 1) & (0, 0) & (1, 0) & (2, 1) \\ \lambda & 1309.82 & 1307.54 & 1299.96 & 1296.78 & 1294.47 & 1283.88 & 1287.09 \end{array}$$

IX.  $Q^1\Pi_u \leftarrow X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (66.24):

$$(v', v'') \quad (1, 1) \quad (0, 0) \\ \lambda \quad 1255.94 \quad 1253.45$$

XI.  $b^1\Sigma_u^- \rightarrow X^1\Sigma_g^+$  System

Band heads,  $\lambda$  (74.44, 67.29):

$v', v''$	0	1	2	3	4
0		3617.9	3721.5	3830.4	3944.9
1		3541.0	3640.2		
2					3767.2

XII.  $B^1\Pi_g \rightarrow A^1\Pi_u$  System

Band heads,  $\lambda$  (73.42):

$$(v', v'') \quad (0, 2) \quad (1, 2) \quad (0, 0) \quad (1, 0) \\ \lambda \quad 6674.0 \quad 6517.8 \quad 6414.0 \quad 6269.7$$

XIII.  $c(^3\Pi_u) \rightarrow b(^3\Pi_g)$  System

Band heads,  $\lambda$  (67.29, 67.27, 64.23):

$v', v''$	$\lambda$			$v', v''$	$\lambda$		
0, 0	10047.5	9934.7	9784.9	2, 0	8924.6	8829.2	8716.8
1, 0	9449.2	9345.8	9218.3	3, 1	8875.4	8786.5	8673.6
2, 1	9389.7	9289.5	9159.1	4, 2	8829.2	8738.9	8622.0
3, 2	9325.8	9218.3	9105.0	5, 3	8786.5	8693.3	8585.7
4, 3	9269.6	9159.2	9047.3	6, 4	8738.9	8648.1	8537.4

SPECTROSCOPIC CONSTANTS

Molecule P<sub>2</sub>

State	T <sub>e</sub>	$\omega_e$	$x_e \omega_e$	B <sub>e</sub>	$\alpha_e \times 10^3$	D <sub>e</sub> × 10 <sup>6</sup>	r <sub>e</sub>	Remarks	Bibliography
S <sup>1Σ<sup>+</sup></sup>	81843.6	(a)	-	0.2783 (d)	-	-	1.978 <sup>(e)</sup>		(66.24)
Q <sup>1Π<sub>u</sub></sup>	80169.2	(a) 618(b)	-	-	-	-	-		(66.24)
N <sup>1Σ<sup>+</sup></sup>	77286.8	701.2	(29.70)	0.29845	5.11	3.1	1.910		(66.24)
M <sup>1Σ<sup>+</sup></sup>	73845.7	678.5	3.0	0.2786	1.6	-	1.977		(66.24)
K <sup>1Π<sub>u</sub></sup>	72288.5	713	5.5	0.2704 (d)	-	-	2.006 <sup>(e)</sup>		(66.24)
I <sup>1Π<sub>u</sub></sup>	68849.4	-	-	0.2541 (d)	-	2.5	2.070 <sup>(e)</sup>		(66.24)
G <sup>1Σ<sup>+</sup></sup>	66313.43	694.12	4.18	0.2973	1.95	2.25	1.913		(66.24, 55.19)
E <sup>1Π<sub>u</sub></sup>	59446.28	700.66	2.92	0.2807 (d)	-	1.84	1.969 <sup>(e)</sup>		(66.24, 55.19)
B <sup>1Π<sub>g</sub></sup>	50223.30	391.3	16.2	0.2300	6.0	3.3	2.176		(73.42)
C <sup>1Σ<sup>+</sup></sup>	46941.33	473.93	2.340	0.24211	1.75	2.57	2.1204	(c)	(66.24)
A <sup>1Π<sub>g</sub></sup>	34515.34	618.78	2.92	0.2752	1.70	2.2	1.9889		(73.42, 58.21)

## SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^5$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$c(^3\Pi_u)$	$10180 + x_1$ $10038 + x_2$ $9915 + x_3$	$640(f)$	4.0						(67.29)
$b(^3\Sigma_u^-)$	$28507.74$	$604.48$	2.2	$0.2583$	1.4	1.6			$(74.44, 73.43,$ $67.29)$
$b(^3\Pi_g)$	$x_1, x_2, x_3$	$562$	3.6						(67.29)
$x(^1\Sigma_g^+)$	0	$780.89$	2.820	$0.30356$	1.43	1.88	$1.8937$	(g)	$(73.43, 67.31,$ $66.24)$

(a)  $T_e + G'(0)$ ; (b)  $\Delta G_{1/2}$ ; (c)  $y_{e\omega_e} = 0.0066 \text{ cm}^{-1}$ ; (d)  $B_o$ ; (e)  $r_o$ ; (f) v uncertain;

(g)  $y_{e\omega_e} = -0.005511 \text{ cm}^{-1}$

Dissociation energy =  $5.04 \pm 0.11 \text{ eV}$ ,  $147.5 \text{ kcal/mole}$ ,  $40651 \text{ cm}^{-1}$  (68.34).

Perturbations and General Information

Many of the vibrational levels of the C<sup>1</sup> $\Sigma_u^+$  state are strongly perturbed (50.18, 50.17, 32.4).

Many of the levels of the E<sup>1</sup> $\Pi_u$  state are perturbed (66.24).

Predissociation of the C<sup>1</sup> $\Sigma_u^+$  state, by a <sup>3</sup> $\Sigma_u^+$  state, is observed at v = 10, J = 58 and v = 11, J = 34. A second predissociation is observed at v = 19 (66.24).

A region of diffuse absorption at 1425 $\text{\AA}$  probably belongs to the I - X system.

Levels of the K<sup>1</sup> $\Pi_u$  state are diffuse (maximum at v = 3, 4), probably due to predissociation.

Potential energy curves - RKRV potentials (70.36):

State	v	U+T <sub>e</sub> (cm <sup>-1</sup> )	r <sub>min</sub> ( $\text{\AA}$ )	r <sub>max</sub> ( $\text{\AA}$ )
E <sup>1</sup> $\Pi_u$	0	59795.9	1.914	2.025
	1	60490.9	1.879	2.073
	2	61179.3	1.854	2.106
	3	61862.2	1.836	2.135
	4	62540.8	1.821	2.160
G <sup>1</sup> $\Sigma_u^+$	0	66659.4	1.860	1.972
	1	67341.8	1.825	2.020
	2	68016.9	1.800	2.054
	3	68683.4	1.782	2.084
	4	69341.3	1.767	2.111
	5	69990.7	1.754	2.136
	6	70631.2	1.742	2.160
K <sup>1</sup> $\Pi_u$	0	72643.6	1.966	2.076
	1	73345.3	1.932	2.125
	2	74036.0	1.911	2.161
	3	74728.1	1.895	2.193
	4	75398.1	1.864	2.194
	5	76078.2	1.857	2.232
M <sup>1</sup> $\Sigma_u^+$	0	74184.2	1.922	2.035
	1	74856.4	1.886	2.083
	2	75523.5	1.862	2.118
	3	76182.5	1.842	2.146
	4	76836.6	1.828	2.173

State	v	U+T <sub>e</sub> (cm <sup>-1</sup> )	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)
N <sup>1Σ<sub>+</sub></sup> <sub>u</sub>	0	77286. 8	1. 858	1. 972
	1	78264. 0	1. 828	2. 032
	2	78844. 0	1. 805	2. 079

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**Pb<sub>2</sub>**

**Pb<sub>2</sub>**

**Methods of Production and Experimental Technique**

**Absorption.**

**Thermal emission.**

**Laser-induced fluorescence.**

**BAND SYSTEMS**

System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
I	A $\approx$ X	Absorption, fluores- cence	7000-6200	R			(72.9, 67.8)
II	B $\approx$ X	Absorption, fluores- cence	5270-4200	R			(72.9, 67.8, 35.4)
III	C $\leftarrow$ X	Absorption	3000-2830	R			(n.p. 10, 67.8)
IV	D $\leftarrow$ X	Absorption	2780-2620	R			(n.p. 10, 67.8)
V	E $\leftarrow$ X	Absorption	2600-2460				(n.p. 10)
VI	F $\leftarrow$ X	Absorption	2450-2300	R			(n.p. 10, 67.8)
VII	G $\leftarrow$ X	Absorption	2167-2136				(n.p. 10)

Molecule Pb<sub>2</sub>

II. B  $\rightleftharpoons$  X SystemBand heads,  $\lambda$  (72.9):

$(v', v'')$	$(3, 2)$	$(3, 1)$	$(3, 0)$	$(4, 1)$	$(4, 0)$	$(5, 0)$
$\lambda$	5058.30	5030.56	5002.95	4991.79	4964.50	4927.56

III. C  $\leftarrow$  X SystemMost intense band heads,  $\lambda$  (n.p. 10):

$\lambda$	3003.1	2942.3	2931.3	2920.4	2911.0	2901.0
Intensity	10	4	5	6	7	7

V. E  $\leftarrow$  X System

Most intense ultraviolet system, with several bands converging (n.p. 10).

VI. F  $\leftarrow$  X SystemMost intense band heads,  $\lambda$  (Intensity) (n.p. 10):

$\lambda$	2435.7	2430.4	2417.4	2410.1	2403.4	2397.0	2390.7
Intensity	9	10	7	6	6	5	5

## SPECTROSCOPIC CONSTANTS

State	T <sub>e</sub>	ω <sub>e</sub>	x <sub>e</sub> ω <sub>e</sub>	B <sub>e</sub>	α <sub>e</sub> × 10 <sup>3</sup>	D <sub>e</sub> × 10 <sup>6</sup>	r <sub>e</sub>	Remarks	Bibliography
B	19490.3	161.64	1.036					(a)	(72.9)
A	14465.5	162.4	0.4						(72.9)
X	0	119.1	0.35						(72.9)

(a)  $y_{e^w e} = 0.0055 \text{ cm}^{-1}$

Dissociation energy =  $0.8 \pm 0.2 \text{ eV}$ ,  $18.5 \text{ kcal/mole}$ ,  $6450 \text{ cm}^{-1}$

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Pd<sub>2</sub>

Pd<sub>2</sub>

Spectroscopic Constants

Dissociation energy =  $1.13 \pm 0.21$  eV, 26 kcal/mole,  $9114 \text{ cm}^{-1}$  (69.3).

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$\text{Po}_2$

$\text{Po}_2$

Methods of Production and Experiments . Technique

Emission from an electrodeless discharge.

Band Systems

Emission, degrading R, has been observed in the region 5130-3600Å.

## SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$(0_u^+)$	25149.3	108.532	0.4417						
$x(0_g^+)$	0	155.715	0.3353					(a)	

(a)  $y_e \omega_e = -0.0003226 \text{ cm}^{-1}$

Dissociation energy =  $1.89 \pm 0.1 \text{ eV}$ ,  $43.5 \text{ kcal/mole}$ ,  $15244 \text{ cm}^{-1}$ .

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Pr<sub>2</sub>

Pr<sub>2</sub>

Spectroscopic Constants

Dissociation energy =  $1.30 \pm 0.30$  eV, 30 kcal/mole,  $10490 \text{ cm}^{-1}$  (72.1).

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Rb<sub>2</sub>Methods of Production and Experimental Technique

## Absorption.

Emission from a discharge in Rb vapor, from a discharge in a heat pipe.

## Laser-induced fluorescence.

## BAND SYSTEMS

System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
I	$A^1\Sigma_u^+ \rightleftharpoons X^1\Sigma_g^+$	Absorption, discharge	11000-8400	R	Max. ~ 10500		(71.20, 34.8)
II	$B^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption, discharge	7350-6400	R	6824. 2(1, 1) 6797. 8(1, 0)		(71.20, 36.10)
III	$C^1\Pi_u \rightleftharpoons X^1\Sigma_g^+$	Absorption, laser- induced fluores- cence	5030-4690	R	4746. 5(10,2)		(71.20, 37.11)
IV	$D \leftarrow X^1\Sigma_g^+$	Absorption	4550-4220	R	4326. 8(10,1) 4288 2(14,0)		(37.11)
V	? $\rightarrow X^1\Sigma_g^+$	Laser- induced fluores- cence	6100-5400			Quasi- continuum	(71.20)
VI	Bands associated with resonance lines (Van der Waals molecules)						(35.7, 32.6)

Molecule Rb<sub>2</sub>

Rb<sub>2</sub>

I. A<sup>1</sup>Σ<sub>u</sub><sup>+</sup> ≈ X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> System

Bands are fragmentary, not analyzed (71.20, 34.8):

$\lambda | 10500 | 9033 | 8989 | 8941 | 8897 | 8852 | 8807 | 8762$

II. B<sup>1</sup>Π<sub>u</sub> ≈ X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> System

Band heads of <sup>85</sup>Rb<sub>2</sub> of greatest intensity,  $\lambda$  (Intensity) (36.10):

(v', v'')	(1, 0)	(2, 0)	(3, 0)	(4, 0)	(6, 1)	(5, 0)
$\lambda$	6797.8	6775.7	6754.5	6734.0	6718.1	6713.2
(Intensity)	10	10	10	10	5	6

III. C<sup>1</sup>Π<sub>u</sub> ≈ X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> System

Band heads of greatest intensity,  $\lambda$  (Intensity) (71.20, 37.11):

(v', v'')	(2, 1)	(3, 0)	(4, 0)	(6, 1)	(9, 2)	(8, 1)	(10, 2)
$\lambda$	4797.1	4775.8	4767.7	4764.6	4754.1	4749.0	4746.5
(Intensity)	9	8	8	8	8	9	10

IV. D ← X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> System

Band heads of greatest intensity,  $\lambda$  (Intensity) (37.11):

(v', v'')	(7, 2)	(8, 2)	(8, 1)	(9, 1)	(10, 1)	(11, 1)	(11, 0)
$\lambda$	4359.3	4351.9	4341.1	4333.8	4326.8	4319.7	4309.2
(Intensity)	8	8	9	9	10	9	9

## SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
D	22777.5	40.42	0.745					(e)	(37.11)
C $^1\Pi_u$	20835.1	36.46	0.124						(37.11)
B $^1\Pi_u$	14662.1	48.05	(a)	(c) 0.191					(36.10)
A $^1\Sigma_u^+$	~11500	-	-						(34.8)
X $^1\Sigma_g^+$	0	57.31	(b) 0.105	(d) ~0.02					(71.20, 37.11, 36.10)

(a)  $\omega_e = 47.78$  for  $^{85}\text{Rb}^{87}\text{Rb}$ , (b)  $\omega_e = 56.98$  for  $^{85}\text{Rb}^{87}\text{Rb}$ , (c)  $x_e \omega_e = 9.188$  for  $^{85}\text{Rb}^{87}\text{Rb}$ ,

(d)  $x_e \omega_e = 0.103$  for  $^{85}\text{Rb}^{87}\text{Rb}$ , (e)  $y_e \omega_e = -0.00144$

Dissociation energy =  $0.47 \pm 0.05$  eV, 10.8 kcal/mole,  $3790 \text{ cm}^{-1}$ .

## Rb<sub>2</sub>

### Perturbations and General Information

Radiation in the region 6100-5400 Å due to transfer from the C state into an unidentified state followed by transitions to high-lying and continuum levels of the ground state (71.20).

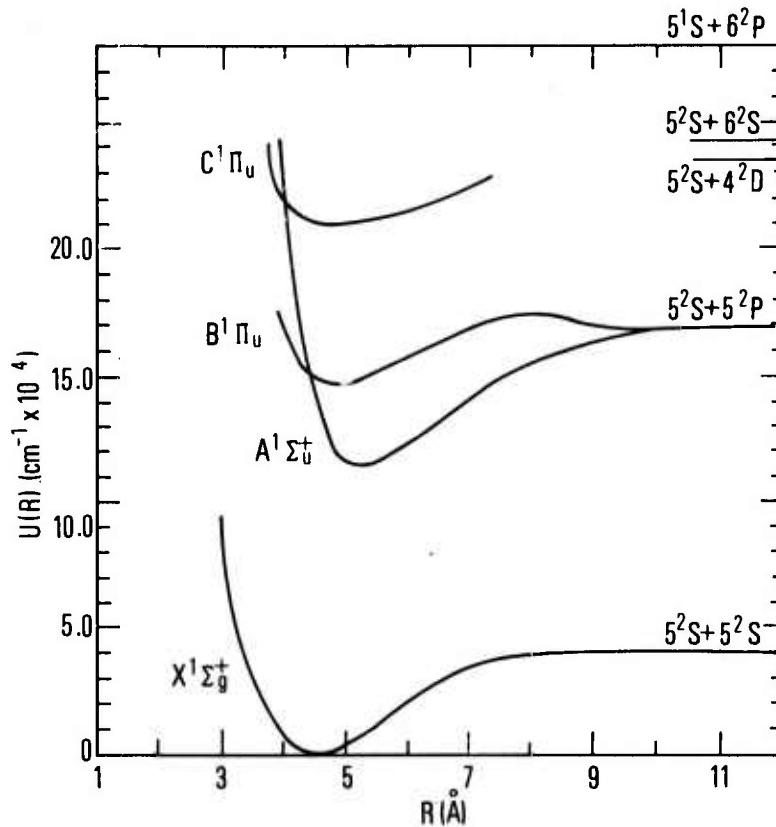
Predissociation of the C state caused by crossing of A state (71.20).

Radiative lifetimes (70.17):

$$B^1\Pi_u - \tau_r \sim 16 \text{ nsec}$$

$$C^1\Pi_u - \tau_r \sim 61 \text{ nsec}$$

Potential energy curves - empirical (71.20)



Average electric dipole polarizability (534°K)  $68 \pm 7 \times 10^{-24} \text{ cm}^3$  (74.25).

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Rb<sub>2</sub>

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S<sub>2</sub>Methods of Production and Experimental Technique

Absorption: at elevated temperatures, in matrices, after flash photolysis.

Emission: high frequency discharge, microwave discharge, flames.

Fluorescence: excited by OH\*, laser-induced.

## BAND SYSTEMS

System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $v_0, 0$	Remarks	Bibliography
I	$b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$	Photolysis	11055-10920			Observation doubtful	(72.110)
II	$B^3\Sigma_u^- \approx X^3\Sigma_g^-$	Absorption, discharge, fluorescence	7110-2400	R	31689	(a)	{72.104, 68.90, 63.73, 62.69, 60.67, 53.61, 48.54}
III	$C^3\Sigma_u^- - X^3\Sigma_g^-$	Absorption	1870-1650	V	55633. 3		(65.83, 48.56, 48.55, 34.26)
IV	$C'^3\Sigma_u^- - X^3\Sigma_g^-$	Microwave	1860-1760	V	56983. 6	(b)	(62.71)
V	$D^3\Pi_u - X^3\Sigma_g^-$	Absorption	1750-1650	V	58750	(b)	(65.83, 48.55, 34.26)
VI	$B'^3\Pi_{g,i} - A^3\Sigma_u^+$	Discharge, microwaves	8083-7434	V	13447. 7	(c)	(66.86, 64.76, 62.69, 35.28)
VII	$B'^3\Pi_{g,i} - A'^3\Delta_{u,i}$	Discharge, microwaves	7761-6984	V	$^3\Pi_1 - ^3\Delta_2$ -14144. 7 $^3\Pi_2 - ^3\Delta_3$ -14318. 0	(c)	(64.76, 62.69, 35.28)
VIII	$f^1\Delta_g \approx a^1\Delta_g$	Absorption, discharge	3350-2400	R	36743		{70.103, 69.100, 64.78, 64.77, 64.76, 63.75}

Molecule S<sub>2</sub>

## BAND SYSTEMS

System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0,0}$	Remarks	Bibliography
IX	$g^1\Delta_u \rightarrow a^1\Delta_g$	Discharge, microwaves	2130-1880	V	52244.7		(68.93, 62.71)
X	$h^1\Sigma_g^+ \rightarrow b^1\Sigma_g^+$	Discharge, microwaves	2130-1760	V	51401.3	(b)	(68.93, 67.89, 65.83, 62.71)
XI	$i \rightarrow b^1\Sigma_g^+$	Discharge, microwaves	2130-1760	V	55448.3	(b)	(68.93, 65.83, 62.71)
XII	$e^1\Pi_g \rightarrow c^1\Sigma_u$	Discharge	7430-7152	V	13452		(62.69)
XIII	?	Microwaves	1850-1780	V	56077.7	(b)	(67.89)

(a) Numerous perturbations and predissociations. Several bands possess secondary heads.  
 (b) Analysis is uncertain.  
 (c) Predissociates.

Molecule S<sub>2</sub>

I.  $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$  System

Observed in laser emission only (75. L117, 72. 110).

$$\lambda | 11055 | 10975 | 10920$$

II.  $B^3\Sigma_u^- \approx X^3\Sigma_g^-$  System

Band heads of  $^{32}S_2$ ,  $\lambda$  (Intensity) (36.30, 31.22, 31.21):

$v', v''$	0	1	2	3	4	5	6
0				3387.0(1)	3469.6(2)	3555.8(3)	3645.2(5) <sup>a</sup>
1			3259.9(2)	3336.7(2)	3417.0(4)	3500.5(5)	3587.4(5)
2		3143.7(1)	3216.1(2)	3290.7(3)	3369.6(4)	3451.0(2)	
3	3033.1(1)	3101.5(1)	3171.5(2)	3244.7(3)	3321.2(1)		
4	2997.0(1)	3063.6(3)	3132.4(3)	3203.2(2)			
5	2960.1(2)	3024.3(4)	3091.7(5)	3161.1(1)			
6	2926.6(2)	2989.7(4) <sup>a</sup>	3054.9(3)				

<sup>a</sup> Bands possessing weak secondary heads

Isotope studies of  $^{34}S_2$  (70.105).

III.  $C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$  System

Each band possesses from 3 to 6 heads, with a maximum separation between extremes of 1 - 8 Å. Isotope effect has been noted for several bands.

Most intense band heads,  $\lambda$  (Intensity) (65.83, 48.55):

$v', v''$	0	1	2	3	4	5
0	1796.93(9)	1820.46(4)	1844.43(3)	1868.82(1)	1894.50(1)	1919.81(1)
1	1770.75(9)		1816.88(1)	1840.51(1)	1864.65(1)	1889.93(1)
2	1745.57(8)	1768.99(2)				
3	1721.29(5)	1742.89(3)				
4	1697.97(4)	1718.90(2)				
5	1675.39(1)	1695.78(2)	1716.56(1)			
6	1653.60(1)	1673.52(1)	1693.72(1)			

IV.  $C' ^3\Sigma_u^- \rightarrow X ^3\Sigma_g^-$  System

Double-headed bands with separation of  $\sim 14 \text{ cm}^{-1}$  are observed.  
Most intense band heads,  $\lambda$  (Intensity) (62.71):

$(v', v'')$	$(0, 4)$	$(0, 3)$	$(0, 2)$	$(0, 1)$	$(0, 0)$
$\lambda$	1859. 49	1835. 57	1811. 94	1788. 84	1766. 11
(Intensity)	1	2	2	5	4

V.  $D ^3\Pi_u \leftarrow X ^3\Sigma_g^-$  System

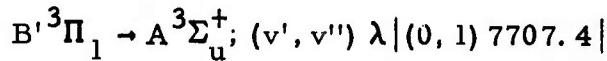
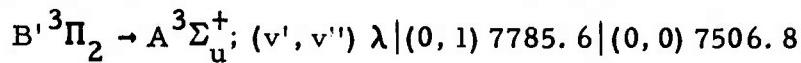
Each band has 9 heads. Most intense band heads of the  $a_3$ ,  $b_3$ , and  $c_3$  series,  $\lambda$  (Intensity) (65.83, 48.55):

$v', v''$	0	1	2	3	4
0	$a_3$ 1709. 95(10)	1729. 18(1)	1750. 93(1)		
	$b_3$ 1702. 37(8)	1723. 44(1)			
	$c_3$ 1694. 60(10)	1715. 83(1)	1737. 02(0)		
1	$a_3$ 1685. 32(4)	1705. 99(3)	1726. 99(0)		
	$b_3$ 1679. 88(4)	1700. 49(3)			
	$c_3$ 1672. 34(6)	1692. 75(4)	1714. 44(0)		
2	$a_3$ 1663. 49(2)	1683. 63(2)	1704. 08(1)	1724. 91(0)	
	$b_3$ 1658. 23(2)	1678. 25(2)	1698. 63(0)		
	$c_3$ 1650. 85(2)	1670. 87(6)		1711. 34(0)	
3	$a_3$	1662. 08(1)	1681. 99(1)		
	$b_3$	1656. 85(0)	1676. 65(1)		1717. 19(0)
	$c_3$	1649. 49(1)	1669. 16(1)		1709. 36(0)

VI.  $B' ^3\Pi_{g,i} \rightarrow A ^3\Sigma_u^+$  System

Two subsystems - because the  $^3\Pi_0$  state is completely predissociated. Only 5 of the 9 possible heads are observed (65.83). Isotope shifts (66.86).

Most intense band heads,  $\lambda$  (66.86, 64.76):



VII.  $B' ^3\Pi_{g,i} \rightarrow A ^3\Delta_{u,i}$  System

Two subsystems - because the  $^3\Pi_0$  state is completely predissociated.

$\lambda$  (64.76, 62.69):



VIII.  $f ^1\Delta_u \approx a ^1\Delta_g$  System

Single-headed bands. Isotope studies (65.82, 65.80).

Most intense band heads,  $\lambda$  (70.103, 64.77)

$v', v''$	0	1	2	3	4	5	6
0					2940.49	2999.74	3060.77
1				2847.52	2903.53		
2			2760.14	2813.24			
3		2677.92	2728.33				
4		2648.34	2697.64				
5		2619.78	2668.02				
6	2546.28	2592.52					
7	2520.56	2565.59					
8	2495.77						
9	2471.77						
10	2448.98						

IX.  $g^1\Delta_u \rightarrow a^1\Delta_g$  System

Single-headed bands. Most intense band heads,  $\lambda$  (Intensity) (68.90, 62.71):

$v'$ , $v''$	0	1	2	3	4	5	6	7
0	1914.06 (9)	1939.89 (9)	1966.08 (9)	1992.63 (7)	2019.68 (6)	2047.24 (4)	2075.24 (3)	2103.73 (2)
1	1884.80 (6)		1934.96 (0)	1960.85 (3)	1987.12 (3)	2013.79 (4)	2040.90 (3)	2068.49 (2)
2			1905.09 (2)			1981.57 (2)	2007.51 (2)	2034.59 (1)
3							1976.15 (0)	2002.01 (1)

X.  $h^1\Sigma_u^+ \rightarrow b^1\Sigma_g^+$  System

Most intense band heads,  $\lambda$  (Intensity) (68.90, 67.89, 65.83):

$v'$ , $v''$	0	1	2	3	4	5	6	7
0	1943.25 (4)	1969.75 (5)	1996.80 (5)	2024.18 (5)	2052.04 (3)	2080.47 (2)		
1				1991.44 (9)	2018.27 (4)	2045.87 (4)	2073.77 (3)	
2			1934.20 (5)		1985.95 (1)	2012.44 (3)	2039.66 (3)	2067.19 (2)
3			1905.09 (2)	1929.42 (1)			2006.75 (1)	2033.33 (1)

XI.  $i \rightarrow b^1\Sigma_g^+$  System

Only a single head is observed. Most intense band heads,  $\lambda$  (Intensity) (68.93, 65.83, 62.71):

$(v', v'')$ $\lambda$ (Intensity)	$(0, 7)$ 1984.52 3	$(1, 8)$ 1979.18 2	$(0, 6)$ 1959.15 0	$(1, 7)$ 1954.07 2	$(0, 5)$ 1934.20 5
$(v', v'')$ $\lambda$ (Intensity)	$(1, 6)$ 1929.44 1	$(0, 4)$ 1909.57 1	$(1, 5)$ 1905.09 2	$(0, 2)$ 1861.73 0	$(1, 1)$ 1811.94 2

## SPECTROSCOPIC CONSTANTS

State	$T_o$ (Observed)	$T_o$ (Calculated)	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^8$	$r_e$	Remarks	Bibliography
i? $^1\Sigma_u^+$ , $^1\Delta_u$	{55448 + b 55448 + a	~64000? ~59900?	-	-	>0.29	-	-	<1.9		(68.93, 65.83, 62.71)
h $^1\Sigma_u^+$	51401.3+a	~59900?	819.6	2.70	>0.29	-	~14.52	<1.89		(65.83, 62.71)
d $^3\Pi_{g,z}$	58750	58750	793.9	4.0	0.3066	-	~16.293	(1.854)	(a)	(69.100, 65.83, 48.55)
C? $^3\Sigma_u^-$	56983.6	56984	-	-	>0.295	-	-	<1.89		(65.83)
g $^1\Delta_u$	52244.7+a	~56700	816.4	2.7	0.3217	1.44	20.0	1.811		(68.83)
C $^3\Sigma_u^-$	55633.3	55633.3	829.15	3.34	0.32196	1.4	22.0	1.810	(b)	(69.99, 65.83, 48.55)
f $^1\Delta_u$	36743.5+a	~41200	438.32	2.70	0.22704	1.78	24.5	2.155	(d)	(70.103, 68.93, 65.83)
e $^1\Pi_g$	13451.8+a	~37000	533.7	(c) -	~0.25	-	-	~2.08		(65.83)
B' $^3\Pi_{g,i}$	14144.7+A'	~36000	-	-	0.244	-	-	2.08	(e)	(65.83, 62.69)
B'' $^3\Pi_u$	31689	31689	434	2.75	0.2244	1.8	23.1	2.168		(63.73)
A' $^3\Sigma_u^+$	697 + A'	~22550	~31700	-	>0.2029	-	-	<2.280		(65.83, 63.73)
c $^1\Sigma_u^-$	c	~23550	477(c)	-	-	-	-	-		(65.83, 62.69)
A' $^3\Sigma_{u,i}$	A'	~21855	488.6	2.63	0.2284	1.40	19.96	2.148	(f)	(62.69)

## SPECTROSCOPIC CONSTANTS

State	$T_o$ (Observed)	$T_o$ (Calculated)	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^8$	$r_e$	Remarks	Bibliography
$b^1\Sigma_g^+$	b	~ 8500	700. 8?	3. 4?	-	-	-	-		(65.83)
$a^1\Delta_g$	a	~ 4500	702. 35	3. 09	0. 29262	1. 73	20. 4	1. 8987		(70.103, 68.93)
$X^3\Sigma_g^-$	$\begin{cases} ^3S_2 \\ ^3D_2 \end{cases}$	0	725. 668	2. 844	0. 29541	1. 58	21. 48	1. 889	(g)	(n.p. 115)
$X^3\Sigma_g^-$	$\begin{cases} ^3S_2 \\ ^3D_2 \end{cases}$	0	704. 026	2. 677	0. 27813	1. 45	19. 59	1. 889	(h)	(n.p. 115)

(a)  ${}^3\Pi_2 - {}^3\Pi_1 \approx 462 \text{ cm}^{-1}$ ; (b)  $\lambda_o = -11.61 \text{ cm}^{-1}$ ,  $\gamma_o = 0.033 \text{ cm}^{-1}$ ; (c)  $\Delta G_{1/2}$ ; (d)  $y_e \omega_e = -0.005 \text{ cm}^{-1}$ ;

(e)  ${}^3\Pi_1 - {}^3\Pi_2 \approx 130 \text{ cm}^{-1}$ ; (f)  ${}^3\Delta_2 - {}^3\Delta_1 \approx 303.5 \text{ cm}^{-1}$ ; (g)  $\lambda_e = 11.82 \text{ cm}^{-1}$ ,  $\gamma_e = -0.0066 \text{ cm}^{-1}$ ; (h)  $\lambda_e = 11.73 \text{ cm}^{-1}$ ,  $\gamma_e = -0.0062 \text{ cm}^{-1}$

Dissociation energy =  $4.4 \pm 0.1 \text{ eV}$ ,  $10.5 \text{ kcal/mole}$ ,  $35300 \text{ cm}^{-1}$  (71.107).

Perturbations and General Information

Perturbations by a  $B''^3\Pi_u$  state are observed for all vibrational levels. There are three perturbations within each branch.

In emission, the predissociation of the  $v'' = 0$  series stops with the (9, 0) band at 2828 Å (31.21).

Higher rotational levels of  $v' = 17$  of the B - X system and all rotational levels of  $v' \geq 18$  are extremely diffuse.

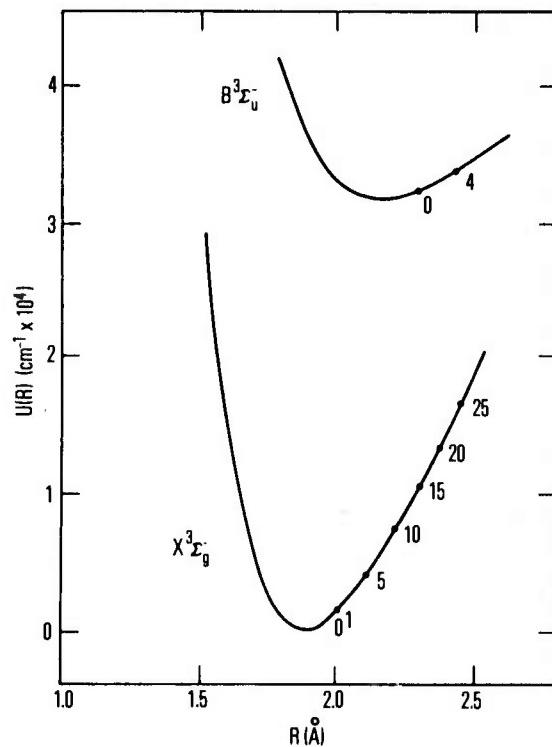
The  $B'^3\Pi_g$  and  $e^1\Pi_g$  states are predissociated at  $v' = 0$  ( $B'^3\Pi_2$  for  $J \geq 34$  and  $B'^3\Pi_2$  for  $J \geq 16$ ) (65.80).

$f^1\Delta_u - a'^1\Delta_g$  systems predissociates for  $v' \geq 10$  (65.80).

Radiative lifetimes (73.111):

$v'$	$\tau$ (nsec)
$B^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$	3      20.7
	4      18.3

Potential energy curves - RKR potential (73.112)



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**Sb<sub>2</sub>**

**Sb<sub>2</sub>**

**Methods of Production and Experimental Technique**

Absorption at elevated temperatures (800-1600°C).

Thermal emission and microwave discharge.

Fluorescence excited by Hg.

**BAND SYSTEMS**

	System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
	I	$A \approx X^1\Sigma_g^+$	Absorption	7500-6000	R			(49.6)
	II	$B \approx X^1\Sigma_g^+$	Absorption	6000-4500	R			(72.9, 49.6)
	III	$D \approx X^1\Sigma_g^+$	Absorption	3400-2830	R	3049.2(6,2)		(67.8, 35.4)
	IV	$F - X^1\Sigma_g^+$	Absorption	2340-2150	R	2222.8(2,1)		(35.4)
	V	?	Microwaves	8400-7200	V	8315.5, 7788.1		(67.8)
	VI	?	Microwaves	4200-3600	R			(67.8)
	VII	?	Microwaves	3000-2900	R		Triplet structure	(67.8)
	VIII	?	Absorption	< 2170	R	2138.6		(35.4)

Molecule Sb<sub>2</sub>

II.  $B \approx X^1\Sigma_g^+$  System

Band heads of  $^{121}\text{Sb}_2$ ,  $\lambda$  (72.9):

(v', v'')	(5, 0)	(4, 0)	(4, 1)	(3, 0)	(3, 1)
$\lambda$	5644.6	5562.0	5496.1	5481.4	5417.5

III.  $D \approx X^1\Sigma_g^+$  System

Most intense bands,  $\lambda$  (Intensity):

(v', v'')	(3, 3)	(4, 3)	(7, 4)	(5, 2)	(8, 4)	(6, 2)
$\lambda$	3134.7	3114.5	3079.0	3068.9	3059.2	3049.2
(Intensity)	4	4	4	4	4	6

IV.  $F \leftarrow X^1\Sigma_g^+$  System

Most intense band heads,  $\lambda$  (Intensity) (35.4):

(v', v'')	(0, 2)	(2, 3)	(0, 1)	(1, 1)	(2, 1)	(2, 0)
$\lambda$	2258.5	2249.7	2244.9	2233.4	2222.8	2209.4
(Intensity)	4	2	5	3	7	5

VIII. Band Groups at 2170A

Most intense bands,  $\lambda$  (Intensity) (35.4):

$\lambda$	2138.6	2126.8	2115.0	2104.3
(Intensity)	3	2	2	2

**Molecule Sb<sub>2</sub>**

## SPECTROSCOPIC CONSTANTS

(a)  $B_2$ , (b)  $D_2$

Dissociation energy =  $2.37 \pm 0.10$  eV, 54.7 kcal/mole,  $19120 \text{ cm}^{-1}$  (73.10).

Perturbations and General Information

D state is vibrationally perturbed (35.4).

D - X system displays predissociation with a peak at 2842 Å. Shorter wavelengths are very diffuse.

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**Sc<sub>2</sub>**

**Sc<sub>2</sub>**

**Spectroscopic Constants**

**Dissociation energy =  $1.12 \pm 0.2$  eV, 25.9 kcal/mole,  $9275 \text{ cm}^{-1}$ .**

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Se<sub>2</sub>Methods of Production and Experimental Technique**Absorption at elevated temperatures.****Emission from a microwave discharge in Se vapor.****Laser-induced fluorescence.**

## BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $v_{0,0}$	Remarks	Bibliography
	I	$B^3\Sigma_u^- - X^3\Sigma_g^-$ $(0_u^+ - 0_g^+)$ $(1_u - 1_g)$	Absorption, fluorescence	6700-3250	R			(72.21, 71.19, 66.11)
	II	$C^3\Sigma_u^- - X^3\Sigma_g^-$ $(0_u^+ - 0_g^+)$ $(1_u - 1_g)$ $(1_u - 0_g^+)$	Absorption	1960-1868	V			(70.17)
	III	?	Absorption	1856-1843				(72.20)
	IV	? - $X^3\Sigma_g^-$ $(1_u - 1_g)$	Absorption	1845-1820				(70.17)
	V	? - $X^3\Sigma_g^-$ $(0_u^+ - 0_g^+)$	Absorption	1826-1812				(70.17)

Molecule Se<sub>2</sub>

**Se<sub>2</sub>**

## BAND SYSTEMS

System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $\nu_{0, 0}$	Remarks	Bibliography
VI	$n \rightarrow a^1 \Delta_g$ $(1_u \rightarrow 2_g)$	oures-nce					(72.20)

Molecule **Se<sub>2</sub>**

I.  $B^3\Sigma_u^- \rightleftharpoons X^3\Sigma_g^- (0_u^+ - 0_g^+, 1_u - 1_g)$  Systems

Origins of bands with greatest intensity,  $\lambda$  (66.11):

(v', v'')	(12, 0)	(13, 0)	(14, 0)	(15, 0)	(16, 0)	(17, 0)	(18, 0)
$\lambda(80\text{Se}_2)$	3483. 4	3457. 5	3432. 1	3407. 3	3383. 3	3360. 0	3337. 3
$\lambda(78\text{Se}_2)$	3479. 8	3453. 4	3427. 8	3402. 9	3378. 6	3355. 1	3332. 4

II.  $C^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$  Systems

a.  $C(0_u^+) \leftarrow X(0_g^+)$

Strong, diffuse bands with no rotational structure,  $\lambda$  (70.17):

(v', v'')	(0, 2)	(0, 1)	(0, 0)	(1, 0)
$\lambda$	1902. 04	1888. 43	1874. 80	1860. 36

b.  $C(1_u) \leftarrow X(1_g)$

Strong bands with sharp rotational structure,  $\lambda$  (70.17):

v', v''	0	1	2	3
0	1896. 49	1910. 43	1924. 50	1938. 7
1	1881. 29			1922. 87
2	1866. 45	1879. 96	1893. 6	
3	1851. 97	1865. 25		

c.  $C(1_u) \leftarrow X(0_g^+)$

Weak bands with sharp structure,  $\lambda$  (70.17):

(v', v'')	(0, 1)	(0, 0)	(1, 0)
$\lambda$	1897. 18	1883. 38	1868. 38

Se<sub>2</sub>

III. ? System

Overlaps a continuum centered at ~ 1845A. Weak bands with sharp structure,  $\lambda$  (70.17):

(v', v'')	(0, 1)	(1, 2)	(0, 0)
$\lambda$	1856. 53	1855. 88	1843. 35

IV. ?  $\leftarrow X^3\Sigma_g^- (1_u \leftarrow 1_g)$  System

Strong bands,  $\lambda$  (70.17):

(v', v'')	(0, 2)	(1, 3)	(0, 1)	(1, 2)	(0, 0)
$\lambda$	1846. 23	1844. 61	1833. 26	1831. 69	1820. 41

V. ?  $\leftarrow X^3\Sigma_g^- (0_u^+ \leftarrow 0_g^+)$  System

Band heads,  $\lambda$  (70.17):

(v', v'')	(0, 0)	(1, 1)	(2, 2)	(3, 3)	(1, 0)	(1, 2)
$\lambda$	1826. 09	1825. 47	1824. 85	1824. 38	1812. 81	1812. 28

SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^4$	$D_e \times 10^8$	$r_e$	Remarks	Bibliography
$1_u$	55276.81	430							(70.17)
$0^+_u$	54752.48	403.9	1.3	0.0924(a)	3. 3				(70.17)
?	54239.41	404							(70.17)
$C(0^+_u)$	533339(c)								
$C(1_u)$	52709.61	428.0	1.22	0.09647 <sup>(a)</sup>	3. 33				(70.17)
$q(1_u)$ <sup>(d)</sup>	26991	155	2	0.055(e)					(72.20)
$n(1_u)$	~25985.2	183	~0.75						(72.20)
$B(0^+_u)$	25980.36	246.291	1.016	0.07048	3. 45	4(f)	2. 4464		(66.11)
$B(1_u)$	25912.45	246.42	1.225	0.07086	5. 53	2(f)	2. 4398		(66.11)
$m(1_u)$	~24000	>154 <sup>(g)</sup>	0.99						(72.20)
$a(2_g)$	~4000	319	0.81						
$X(1_g)$	366.7	387.156	0.964	0.09016	2. 98	2	2. 1630		(71.19, 66.11)

Molecule  $Se_2$

SPECTROSCOPIC CONSTANTS

Molecule  $\text{Se}_2$

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^4$	$D_e \times 10^8$	$r_e$	Remarks	Bibliography
$X(0_g^+)$	0	385.302	0.96363	0.08992	2.88	2.4	2.1659		(71.19, 66.11)

(a)  $B_o$ , (b)  $r_o$ , (c)  $T_o$ , (d) analyzed through perturbation of the B state, (e)  $B_2$ , (f)  $D_o$ , (g)  $\Delta G_{1/2}$

Dissociation energy =  $3.164 \pm 0.002$  eV, 72.9 kcal/mole,  $25518 \text{ cm}^{-1}$  (72.20).

Perturbations and General Information

B(0<sub>u</sub><sup>+</sup>) state is perturbed for all vibrational levels, v ≤ 15 by m, n, and q states. Perturbations for levels of low v are weak (72.20, 63.9).

Both B(0<sub>u</sub><sup>+</sup>) and B(1<sub>u</sub>) states predissociate (63.9).

Ionization potential (I<sub>p</sub>) = 8.88 ± 0.03 eV (69.15).

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Si<sub>2</sub>Si<sub>2</sub>Methods of Production and Experimental TechniqueAbsorption by flash-photolysis in C<sub>6</sub>H<sub>5</sub>SiH<sub>3</sub> or BrSiH<sub>3</sub>.Emission from discharge in SiH<sub>4</sub> and Xe.

## BAND SYSTEMS

System	Transition	Sources	Wavelength Limits	Degrading	Characteristic Bands, $\lambda$	Remarks	Bibliography
I	H <sup>3</sup> $\Sigma_u^-$ - X <sup>3</sup> $\Sigma_g^-$	Flash-photolysis	4526-3863	R	3979. 6(4,1)		(71.6, 63.3, 55.2)
II	L <sup>3</sup> $\Pi_g$ - D <sup>3</sup> $\Pi_u$	Discharge and flash-photolysis	3695-3489	R	3568. 7(0, 1) 3496. 0(1, 1)		(71.6, 55.2)
III	K <sup>3</sup> $\Sigma_u^-$ - X <sup>3</sup> $\Sigma_g^-$	Flash-photolysis	3275-3067	R	3202. 0(1, 0)		(71.6, 63.3)
IV	D <sup>3</sup> $\Pi_u$ - X <sup>3</sup> $\Sigma_g^-$	Flash-photolysis	2900-2700		2882. 84 2795. 80		(70.5)
V	N <sup>3</sup> $\Sigma_u^-$ - X <sup>3</sup> $\Sigma_g^-$	Flash-photolysis	2166-2097	R	2138. 35(0,0)		(70.4, 63.3)
VI	O <sup>3</sup> $\Sigma_u^-$ - X <sup>3</sup> $\Sigma_g^-$	Flash discharge	2200-1800		1874.28(0,0) 1892.21(0,1)		(70.4)
VII	P <sup>3</sup> $\Pi_g$ - D <sup>3</sup> $\Pi_u$	Flash discharge	1870-1900	R	1879. 9(0, 0) 1898. 4(0, 1)		(70.4)

Molecule Si<sub>2</sub>

I. H<sup>3Σ<sub>u</sub><sup>-</sup></sup> - X<sup>3Σ<sub>g</sub><sup>-</sup> System</sup>

Band heads,  $\lambda$  (63.3, 55.2):

v', v''	0	1	2	3	4	5	6
0					4427.6	4526.0	
1				4283.1	4375.8	4471.9	
2					4326.0		
3	3942.1						
4	3900.8	3979.6	4060.9				4414.4
5	3863.4						

II. L<sup>3Π<sub>g</sub></sup> - D<sup>3Π<sub>u</sub> System</sup>

Band heads,  $\lambda$  (71.6, 55.2):

v', v''	0	1	2	3	4
0		3568.7	3634.4	3710.4	3772.3
1		3496.0	3563.1	3632.2	

III. K<sup>3Σ<sub>u</sub><sup>-</sup></sup> - X<sup>3Σ<sub>g</sub><sup>-</sup> System</sup>

Band heads,  $\lambda$  (63.3):

(v', v'')	(0, 0)	(1, 0)	(2, 0)	(3, 0)	(4, 0)
$\lambda$	3248.9	3202.0	3157.8	3115.8	3076.1

IV. D<sup>3Π<sub>u</sub></sup> - X<sup>3Σ<sub>g</sub><sup>-</sup> System</sup>

Several lines have been observed in absorption but have not been identified (70.5):

$\lambda | 2882.8 | 2838.8 | 2795.8 | 2758.8$

$\text{Si}_2$

V.  $\text{N}^3\Sigma_u^- - \text{X}^3\Sigma_g^-$  System

Band heads,  $\lambda$  (70.4):

$v'$ , $v''$	0	1
0	2138.35	2161.78
1	2117.92	
2	2098.53	
3	2079.75	2101.92
4		2083.53

VI.  $\text{O}^3\Sigma_g^- - \text{X}^3\Sigma_g^-$  System

Band heads,  $\lambda$  (70.4):

$v'$ , $v''$	0	1	2
0	1874.28	1892.21	
1	1860.53		189.32
2	1847.22	1864.63	

VII.  $\text{P}^3\Pi_g - \text{D}^3\Pi_u$  System

Two red shaded bands have been observed overlapping the O-X system. They are tentatively assigned as follows:

1879.0(0,0)  
1898.4(0,1)

## SPECTROSCOPIC CONSTANTS

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e$	$\alpha_e \times 10^3$	$D_e \times 10^6$	$r_e$	Remarks	Bibliography
$P^3\Pi_g$	88219								(70.4)
$L^3\Pi_g$	63059.1			0.2370			2.255		(70.4, 55.2)
$O^3\Sigma_u^-$	53341.94	404.2	3.0	0.2225	3		2.327		(70.4, 63.3)
$N^3\Sigma_u^-$	46762.2 i	458.6	4.8	0.2143	2.5		2.344		(70.4, 55.2)
$D^3\Pi_u$	~35000	547.94	2.43	0.2596	1.55		2.155		(70.4, 63.4)
$K^3\Sigma_u^-$	30768.77	462.6	5.95	0.2185	3.16		2.349		(71.6, 70.4) 63.3, 55.2)
$H^3\Sigma_u^-$	(a) 24311.15	275.30	1.99	0.1712			2.6536		(70.4, 63.3)
$X^3\Sigma_g^-$	0	510.98	2.02	0.2390	1.3		2.246		

(a)  $T_o$ Dissociation energy =  $3.35 \pm 0.2$  eV, 75 kcal/mole,  $26168 \text{ cm}^{-1}$ .

Perturbations and General Information

The bands of the K - X and H - X systems exhibit the presence of perturbations.

In the H - X system, the (4, 0) band is sharp, but the (5, 0) band is diffuse and does not appear in emission. All the bands of the K - X system are diffuse.

All the levels above v' = 0, J' = 51 of the L state are predissociated.

The position of the (2, 0) band in the N - X system is displaced somewhat to the red, indicating a perturbation (70.4).

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$\text{Sm}_2$

$\text{Sm}_2$

Spectroscopic Constants

Dissociation energy =  $0.52 \pm 0.22$  eV, 12 kcal/mole,  $4200 \text{ cm}^{-1}$  (72.1).

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$\text{Sn}_2$

$\text{Sn}_2$

Band Systems

Bands in the region 4780-4350 $\text{\AA}$  have been attributed to  $\text{Sn}_2$  but may possibly arise from  $\text{SnCl}_2$  (62.2).

Spectroscopic Constants

Dissociation energy =  $1.99 \pm 0.18$  eV, 45.8 kcal/mole,  $16000 \text{ cm}^{-1}$  (62.1).

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Tb<sub>2</sub>

Tb<sub>2</sub>

Spectroscopic Constants

Dissociation energy = 1.34 ± 0.35 eV, 31 kcal/mole, 11000 cm<sup>-1</sup> (72.1).

Tb<sub>2</sub>

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$\text{Te}_2$

$\text{Te}_2$

Methods of Production and Experimental Technique

Absorption.

Emission from microwave discharge.

Fluorescence, laser-induced fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Band Head, $v_0, 0$	Remarks	Bibliography
	I	$A 0_u^+ \rightarrow X 0_g^+$	Absorption	5190-4250	R			(69.45, 69.43)
	II	$B 0_u^+ \rightarrow X 0_g^+$	Absorption from discharge	6320-3836	R			(69.43, 69.41, 66.36, 42.31, 38.28, 35.16, 27.1)
	III	$B 0_u^+ \rightarrow X 1_g$	Laser fluo- rescence	5300-6050	R			(72.49)

Molecule  $\text{Te}_2$

$\text{Te}_2$

I.  $A\ 0_u^+ \leftarrow X\ 0_g^+$  System ( $^{130}\text{Te}_2$ )

Band origins,  $\lambda$  (69.43):

$v', v''$	0	1	2	3	4
0					
...					
6				5190.0	
7			5089.7	5153.4	
8			5054.8	5117.7	
9			5020.7	5082.6	
10	4868.5		4987.2	5048.4	
11	4837.4			5015.0	
12	4806.9	4864.2			
13	4777.1	4833.7			
14		4803.8			
15	4665.2	4774.9			
16	4637.9				
17	4611.3	4664.2			
18	4585.1	4637.5			
19	4559.6	4611.4			
20		4585.8			

II.  $B\ 0_u^+ \approx X\ 0_g^+$  System ( $^{130}\text{Te}_2$ )

Band origins,  $\lambda$  (69.45, 69.41):

$v', v''$	0	1	2	3
0				
...				
5		4449.1		
6		4418.5	4466.6	
7	4341.8	4388.5	4436.0	
8	4313.2	4359.3	4406.2	
9	4240.5	4285.2	4330.7	
10	4213.7	4257.8	4302.7	
11	4187.5	4231.1		
12	4162.0	4205.0		
13	4137.0	4179.6		
14	4112.6			
15	4088.8			
16	4065.7			
17	4043.1			
18	4021.2			
19	3999.8			
20	3979.1			

$B\ 0_u^+ \approx X\ 0_g^+$  System  $^{128}\text{Te}_2$

Band origins,  $\lambda$  (69.45, 69.41):

$v', v''$	0	1	2	...	30	31	32	33
0								
...								
5					6248.7			
6					6188.6	6271.3		
7			4388.8				6210.7	6294.3
8		4312.9	4359.4					6233.8
9		4284.7	4330.2					6317.7
10		4257.1						
11	4186.4	4230.3						
12	4160.7	4204.0						
13	4135.6	4178.6						
14	4110.9							
15	4087.2							
16	4064.0							
17	4041.3							
18	4019.2							
19	3997.8							
20	3977.0							

III.  $B\ 0_u^+ - X\ 1_g^-$  System

Band heads,  $\lambda$  (72.58):

	$^{128}\text{Te}_2$	$^{130}\text{Te}_2$
$v'', v'$	0	0
0		
...		
5	5350.0	
6	5421.1	
7	5493.6	5492.7
8	5567.9	5566.1
9	5643.8	5641.6
10	5721.6	5718.8
11	5800.9	5797.8
12	5882.3	5878.7
13	5965.6	5961.1
14	6050.8	6045.5
15	6138.2	
16	6227.7	

SPECTROSCOPIC CONSTANTS

Molecule  $\text{Te}_2$

State	$T_e$	$\omega_e$	$x_e \omega_e$	$B_e \times 10^2$	$\alpha_e \times 10^4$	$D_e \times 10^9$	$r_e$	Remarks	Biography
$^{130}\text{Te}_2$									
$B\ 0_u^+$	22207.4	162.3	0.45	3.254	1.25		2.8244	$y_e \omega_e = -11.09 \times 10^{-3}$	(72.48, 69.43)
$A\ 0_u^+$	19450.8	143.6	0.45	3.124	1.30		2.8824	$y_e \omega_e = -3.892 \times 10^{-3}$	(72.48, 69.43)
$X\ 1_g$	2234	250.00	0.547	3.968(a)	1.06(a)				(72.49, 69.43)
$X\ 0_g^+$	0	247.07	0.515	3.968	1.06	4.4	2.5774	$y_e \omega_e = -0.55 \times 10^3$	(72.48, 69.43)
$^{128}\text{Te}_2$									
$B\ 0_u^+$	22285.6(b)			3.3121	1.41		2.82442		(72.48, 69.43)
$A\ 0_u^+$	19450			3.1740	1.32		2.88226		(72.48, 69.43)
$X\ 1_g$	2228.5	251.26	0.536	4.0299(a)	1.03(a)				(72.48, 69.45)
$X\ 0_g^+$	0			4.0299	1.03	4.1	2.55766		(72.48, 69.45)

$\text{T}^{-6}$

Molecule Te<sub>2</sub>

## SPECTROSCOPIC CONSTANTS

$\text{Te}_2$

Perturbations and General Information

RKR potential energy curve (n.p. 50) for  $^{128}\text{Te}_2 \times 0_g^+$  state:

$T_e = 0 \text{ cm}^{-1}$	v	$T_e + E(v) \text{ cm}^{-1}$	$r_{\min} (\text{\AA})$	$r_{\max} (\text{\AA})$
	0	124. 35	2. 51335	2. 60548
	1	372. 26	2. 48249	2. 64234
	2	619. 12	2. 46205	2. 66878
	3	864. 92	2. 44591	2. 69096
	4	1109. 65	2. 43229	2. 71065
	5	1353. 33	2. 42037	2. 72867
	6	1595. 94	2. 40971	2. 74547
	7	1837. 49	2. 40000	2. 76133
	8	2077. 96	2. 39108	2. 77646
	9	2317. 36	2. 38286	2. 79084
	10	2555. 68	2. 37513	2. 80484
	11	2792. 92	2. 36782	2. 81846
	12	3029. 09	2. 36095	2. 83165
	13	3264. 16	2. 35441	2. 84456
	14	3498. 15	2. 34819	2. 85715
	15	3731. 05	2. 34227	2. 86953

RKR potential energy curve (n.p. 50) for  $^{128}\text{Te}_2 A 0_u^+$  state:

$T_e = 19450 \text{ cm}^{-1}$	v	$T_e + E(v) \text{ cm}^{-1}$	$r_{\min} (\text{\AA})$	$r_{\max} (\text{\AA})$
	0	72. 24	2. 82474	2. 94564
	1	216. 01	2. 78550	2. 99546
	2	358. 83	2. 75988	3. 03171
	3	500. 67	2. 73987	3. 06242
	4	641. 50	2. 72311	3. 08994
	5	781. 30	2. 70854	3. 11533
	6	920. 05	2. 69557	3. 13918
	7	1057. 72	2. 68383	3. 16188
	8	1194. 28	2. 67307	3. 18367
	9	1329. 73	2. 66317	3. 20455
	10	1464. 02	2. 65389	3. 22501
	11	1597. 14	2. 64511	3. 24506
	12	1729. 07	2. 63686	3. 26464
	13	1859. 78	2. 62900	3. 28393
	14	1989. 24	2. 62153	3. 30290
	15	2117. 43	2. 61435	3. 32167

**Te<sub>2</sub>**

RKR potential energy curve (n.p. 50) for <sup>128</sup>Te<sub>2</sub> B 0<sub>u</sub><sup>+</sup> state:

T <sub>e</sub> = 22285. 6 cm <sup>-1</sup>	v	T <sub>e</sub> + E(v) cm <sup>-1</sup>	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)
	0	81. 68	2. 77021	2. 88390
	1	244. 31	2. 73361	2. 93102
	2	405. 92	2. 70967	2. 96521
	3	566. 44	2. 69099	2. 99420
	4	725. 80	2. 67543	3. 02028
	5	883. 93	2. 66201	3. 04448
	6	1040. 77	2. 65009	3. 06729
	7	1196. 24	2. 63915	3. 08889
	8	1350. 28	2. 62870	3. 10929
	9	1502. 76	2. 61904	3. 12893
	10	1653. 68	2. 60899	3. 14728
	11	1803. 11	2. 60141	3. 16717
	12	1950. 68	2. 59302	3. 18565
	13	2096. 49	2. 58499	3. 20395
	14	2240. 49	2. 57882	3. 22345
	15	2382. 58	2. 57212	3. 24213

Franck-Condon factors for <sup>128</sup>Te<sub>2</sub> (A 0<sub>u</sub><sup>+</sup> - X 0<sub>g</sub><sup>+</sup>) (n.p. 50):

	12	13	14	15	16	17	18	19
0	4. 985-2	6. 959-2	8. 846-2	1. 032-1	1. 110-1	1. 102-1	1. 014-1	8. 679-2
1	7. 975-2	7. 178-3	5. 109-2	2. 559-2	5. 839-3	2. 330-4	1. 094-2	3. 319-2
2	3. 035-2	7. 032-3	4. 068-4	1. 415-2	3. 767-2	5. 356-2	5. 064-2	3. 155-2
3	4. 838-4	1. 598-2	3. 871-2	4. 614-2	3. 100-2	8. 307-3	2. 854-4	1. 440-2
4	2. 969-2	4. 213-2	2. 891-2	6. 186-3	1. 449-3	1. 988-2	3. 861-2	3. 526-2
5	3. 601-2	1. 414-2	2. 368-6	1. 316-2	3. 354-2	3. 128-2	9. 981-3	2. 531-4
6	7. 044-3	1. 933-3	2. 217-2	3. 304-2	1. 643-2	2. 123-4	1. 101-2	3. 076-2
7	3. 998-3	2. 552-2	2. 833-2	7. 349-3	1. 782-3	2. 138-2	2. 942-2	1. 135-2
8	2. 536-2	2. 501-2	3. 738-3	5. 140-3	2. 536-2	2. 256-2	2. 672-3	5. 871-3
9	2. 428-2	3. 104-3	6. 396-3	2. 556-2	1. 740-2	2. 713-4	1. 184-2	2. 638-2
10	4. 517-3	5. 263-3	2. 444-2	1. 540-2	2. 557-6	1. 458-2	2. 409-2	6. 246-3

Franck-Condon factor followed by factor of ten

$\text{Te}_2$

Franck-Condon factors for  $^{128}\text{Te}_2$  ( $B\ 0_u^+ - X\ 0_g^+$ ) (n.p. 50):

	9	10	11	12	13	14	15	16
0	8.506-2	1.101-1	1.267-1	1.305-1	1.208-1	1.001-1	7.702-2	5.374-2
1	8.231-2	5.196-2	1.833-2	5.264-4	8.427-3	3.676-2	7.006-2	9.305-2
2	7.989-3	1.866-3	2.622-2	5.616-2	6.270-2	4.059-2	1.115-2	1.710-4
3	1.719-2	4.769-2	5.101-2	2.326-2	6.824-4	1.165-2	4.208-2	5.623-2
4	4.911-2	3.233-2	3.279-3	7.950-3	3.754-2	4.508-2	1.981-2	1.478-4
5	2.209-2	1.318-5	1.961-2	4.190-2	2.498-2	8.072-4	1.316-2	4.003-2
6	1.247-4	2.365-2	3.789-2	1.228-2	1.716-3	2.766-2	3.619-2	1.062-2
7	2.161-2	3.507-2	8.070-3	5.026-3	3.186-2	2.546-2	1.000-3	1.360-2
8	3.429-2	8.942-3	5.096-3	3.117-2	1.933-2	4.950-5	2.135-2	3.063-2
9	1.396-2	2.415-3	2.848-2	1.842-2	2.691-4	2.322-2	2.494-2	1.082-3
10	3.614-5	2.312-2	2.132-2	3.220-6	2.129-2	2.269-2	2.589-4	1.739-2

Franck-Condon factor followed by factor of ten

Perturbations of the  $v=0$  level of the  $B\ 0_u^+$  state have been observed.

Ionization cross sections =  $17.46 \pm 0.48 \times 10^{-6} \text{ cm}^2$  (66.37).

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$\text{Th}_2$

$\text{Th}_2$

Spectroscopic Constants

Dissociation energy =  $2.95 \pm 0.35$  eV, 68 kcal/mole,  $24000 \text{ cm}^{-1}$  (69.1).

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Ti<sub>2</sub>

Ti<sub>2</sub>

Spectroscopic Constants

Dissociation energy =  $1.15 \pm 0.17$  eV, 28.3 kcal/rad, 9000 cm<sup>-1</sup> (69.2).

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High Temp. Sci. 1, 258-67

Tl<sub>2</sub>

Tl<sub>2</sub>

Methods of Production and Experimental Technique

Absorption.

Emission from a hollow cathode and a King furnace.

Band Systems

Five groups of bands have been observed in emission and absorption (65.5, 65.4, 31.2, 31.1).

I. "Red System" - 6500-4900Å

$\lambda$  in emission (65.5):

v', v''	0	1	2	3	4
0	6320.3	6375.5	6428.4	6483.0	6537.2
1	6285.4	6339.1	6393.0		
2	6252.0				

The conclusions on the origin of this band system are uncertain. Initial investigation gives  $\omega' \sim 88 \text{ cm}^{-1}$  and  $\omega'' \approx 136 \text{ cm}^{-1}$  (65.5).

II. 4635-3680Å System

## Emission

In emission, the band head appears to be at  $\lambda \sim 3770.7\text{\AA}$ , with band maxima at:

$$\lambda = 4635 | 4405 | 4308 | 4237 | 4187 | 4133 | 4047 | 4004$$

diffuse and weak maxima at:

$$\lambda = 3923 | 3857 | 3800$$

## Absorption

Extensive tables of lines seen in absorption (4400-4200Å) are given in (65.5). There are two tentative assignments given to some of them.

## Assignment I:

v', v''	0	1	2	3	4	5	6	7	8
0	4269.9	4287.1	4302.2	4322.2	4340.3				
1		4263.7		4299.1	4360.2	4335.4	4354.2	4372.4	4390.3
2			4251.6	4276.8	4293.9				
3				4255.3	4271.9				
4					4250.8				

Tl<sub>2</sub>

Assignment II:

v', v''	0	1	2	3	4	5	6	7
0	4400.2	4419.0						
1		4394.3	4412.6	4431.9				
2		4370.2		4405.5	4425.1			
3					4401.9	4420.4		
4						4396.0	4414.2	
5						4372.4	4390.3	4408.7

III. 3776-3260 $\text{\AA}$  System

Bands are symmetrical around the lines at 3529 and 3519 $\text{\AA}$ . Maxima at  $\sim 3600\text{\AA}$ .

IV. 2850-2740 $\text{\AA}$  System

Bands are asymmetrical around the 2768 $\text{\AA}$  line with an apparent head at 2766.3 $\text{\AA}$ .

V. Visible Continua - 2768 $\text{\AA}$  System

This system arises from the broadening of the lines 3230, 3092, 2922-2919 $\text{\AA}$ . Maxima at  $\lambda \sim 3446 | 3156 | 3050\text{\AA}$ .

Spectroscopic Constants

Dissociation energy = <0.9 eV, <21 kcal/mole, <7300 cm<sup>-1</sup> (57.3).

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Tm<sub>2</sub>

Tm<sub>2</sub>

Spectroscopic Constants

Dissociation energy = 0.52 ± 0.17 eV, 12 kcal/mole, 4200 cm<sup>-1</sup> (72.2).

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U<sub>2</sub>

U<sub>2</sub>

Spectroscopic Constants

Dissociation energy =  $1.73 \pm 0.43$  eV, 40 kcal/mole,  $14000 \text{ cm}^{-1}$  (69.1).

U-1

U<sub>2</sub>

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High Temp. Sci. 1, 258-67

v<sub>2</sub>

v<sub>2</sub>

Spectroscopic Constants

Dissociation energy = 2.49 ± 0.13 eV, 57.5 kcal/mole, 20100 cm<sup>-1</sup> (69.1).

v-1

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Xe<sub>2</sub>

Xe<sub>2</sub>

Methods of Production and Experimental Technique

Absorption.

Emission from electron beam discharge, laser pumping,  $\alpha$  particles, x rays.

BAND SYSTEMS

System	Transition	Sources	Wavelengths (Å)	Degrading	Band Head, $v_{0,0}$	Remarks	Bibliography
I	?	Electron beam, X rays	5000-2600			Continuum	(67.7)
II	$^1\text{S}_u^+ - X^1\text{S}_g^+$ $(0_u^+ - 0_g^+)$ $(1_u - 0_g^+)$	Electron beam	2250-1470			Continuum	(74.33, 72.14, 65.4, 55.3, 55.2)
III	$^1\text{S}_u^+ - X^1\text{S}_g^+$ $(0_u^+ - 0_g^+)$	Electron beam	1305-1295				(74.33, 72.14)
IV	$^1\text{S}_u^+ - X^1\text{S}_g^+$ $(0_u^+ - 0_g^+)$	Electron beam	1207-1192				(74.33, 72.14)
V	$^3\text{S}_u^+ - X^1\text{S}_g^+$ $(1_u - 0_g^+)$	Electron beam	1192-1191				(74.33, 72.14)

Molecule Xe<sub>2</sub>

Xe<sub>2</sub>

II.  $^1, ^3 \Sigma_u^+ \rightleftharpoons X ^1 \Sigma_g^+ (0_u^+, ~ ^1_u - 0_g^+)$  Systems

Upper state correlated to  $5p^6 \ ^1S_0 + 6s(3/2)_1^0$  (74.33, 72.14).

III.  $\frac{^1\Sigma_u^+ - X ^1\Sigma_g^+}{(0_u^+ - 0_g^+)} \text{ System}$

Upper state correlated to  $5p^6 \ ^1S_0 + 6s'(1/2) \ ^0_1$  (74.33, 72.14).

IV.  $^1\Sigma_u^+ \leftarrow X ^1\Sigma_g^+ (o_u^+ - o_g^+)$  System

Upper state correlated to  ${}^5\text{p}^6 \ {}^1\text{S}_0 + {}^5\text{d}(3/2) \ {}^0_1$  (74.33, 72.14).

## SPECTROSCOPIC CONSTANTS

State	T <sub>e</sub>	ω <sub>e</sub>	x <sub>e</sub> ω <sub>e</sub>	B <sub>e</sub>	α <sub>e</sub> × 10 <sup>3</sup>	D <sub>e</sub> × 10 <sup>6</sup>	r <sub>e</sub>	Remarks	Bibliography
X <sup>1Σ<sup>+</sup><sub>g</sub></sup> (0 <sup>+</sup> <sub>g</sub> )	0	~21.26	~0.75	~0.013	~0.4		~4.45	y <sub>e</sub> ω <sub>e</sub> ~ 0.008	(70.9)

Dissociation energy ~  $2.4 \times 10^{-2}$  eV, 0.55 kcal/mole, 192.02 cm<sup>-1</sup> (70.9).

## Xe<sub>2</sub>

### Perturbations and General Information

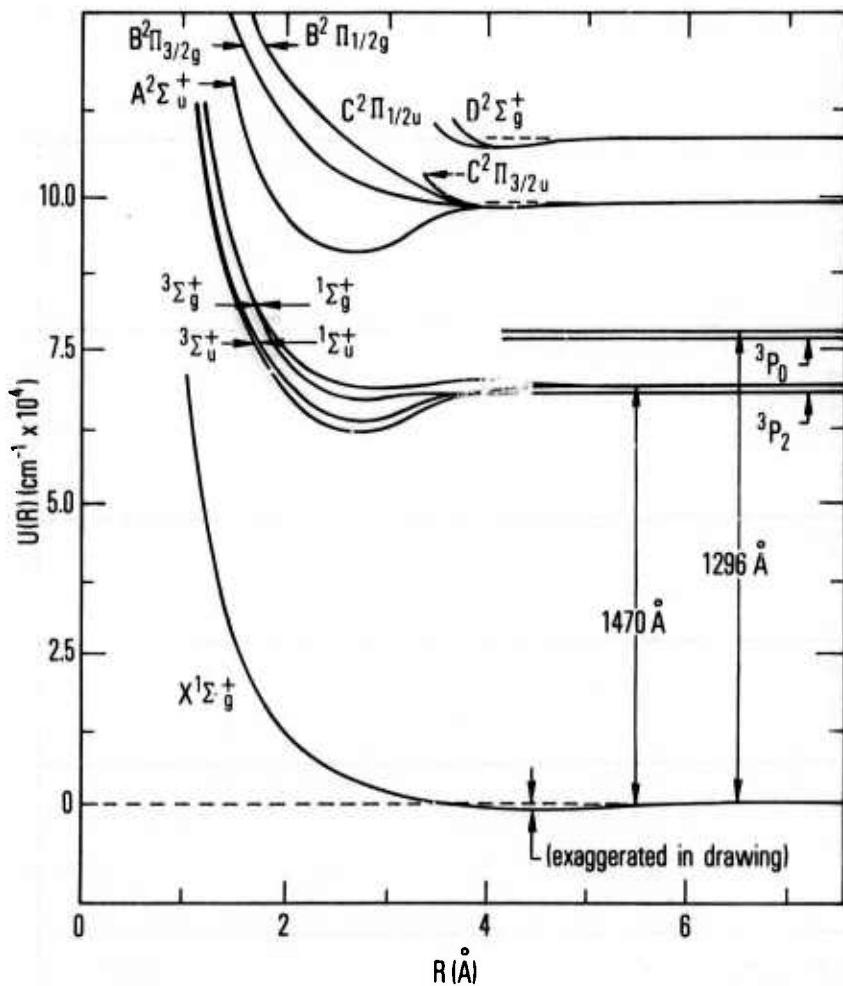
Quenching of Xe<sub>2</sub>  $^1,3\Sigma_u^+$  by Xe:  $\sigma \approx 10^{-17} \text{ cm}^2$  (73.25).

Laser action observed on the  $^1,3\Sigma_u^+ \rightarrow X^1\Sigma_g^+$  transition at  $1720 \pm 10\text{\AA}$  (74.36, 74.31, 74.30, 73.28, 73.23, 73.22, 73.21, 73.20, 73.19, 73.18).

Radiative lifetime of  $^1,3\Sigma_u^+ - X^1\Sigma_g^+$

$$\begin{aligned}\tau &= 23 \text{ nsec (74.32)} \\ &= 130 \text{ nsec (73.18).}\end{aligned}$$

Potential energy curves - estimated (70.10):



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Y<sub>2</sub>

Y<sub>2</sub>

Spectroscopic Constants

Dissociation energy =  $1.62 \pm 0.22$  eV, 37.3 kcal/mole,  $13050\text{ cm}^{-1}$ .

Y-1

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$\text{Yb}_2$

$\text{Yb}_2$

Methods of Production and Experimental Technique

Knudsen cell effusion.

Spectroscopic Constants

Dissociation energy =  $4 \pm 4$  eV, 92 kcal/mole,  $32000 \text{ cm}^{-1}$  (72.3).

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$Zn_2$

$Zn_2$

Methods of Production and Experimental Technique

Absorption.

Emission (Tesla coil, hollow cathode).

Fluorescence.

BAND SYSTEMS

	System	Transition	Sources	Wavelength Limits	Degrading	Maximum ( $\lambda$ ) in Emission	Remarks	Bibliography
	I		Emission	5350-3890		4450	Continuum	(31.6, 31.5)
	II		Emission	3893-3776		3787	Continuum	(31.6, 31.5)
	III		Emission Absorption	3763-2936		3688	Continuum	(31.6, 31.5, 29.2)
	IV		Absorption Emission Fluores- cence	3073-2002		2550	Continuum	(31.6, 31.5, 31.4, 29.2)

Molecule  $Zn_2$

$Zn_2$

III. 3763-2936 $\text{\AA}$  System

Emission

In emission maximum is at  $\lambda = 3688\text{\AA}$  (31.6, 31.5) and line broadens at  $3076\text{\AA}$  (31.6, 31.5).

Bands superimposed	$\lambda$	3749	3724	3706	3688	3575	3522	3483
		3454	3431	3411	3052			

Absorption

In absorption bands are without structure and maxima is at  $\sim 3050\text{\AA}$  (31.6, 29.2).

IV. 3073-2002 $\text{\AA}$  System

Emission (31.6, 31.5)

In emission continuous bands are  $2826-2035\text{\AA}$ , maximum is at  $2550\text{\AA}$ , line broadens at  $2139\text{\AA}$ , and diffuse bands are at  $\lambda \sim 2002\text{\AA}$ .

Absorption (31.6, 29.2)

In absorption continuous bands are at  $2550-2002\text{\AA}$ , maxima are at  $\lambda = 2139$ , 2064, and  $2002\text{\AA}$ , and the line broadens at  $2139\text{\AA}$ .

Fluorescence (31.3)

Numerous bands in the region  $3073-2456\text{\AA}$ .

Spectroscopic Constants

Dissociation energy = 0.25 eV(?), 6 kcal/mole(/),  $2100 \text{ cm}^{-1}$ .

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